New Horizons in Ab Initio Nuclear Structure Theory

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

New Era of Low-Energy Nuclear Physics

Experiment

new facilities and experiments to produce nuclei far-off stability and study a range of observables

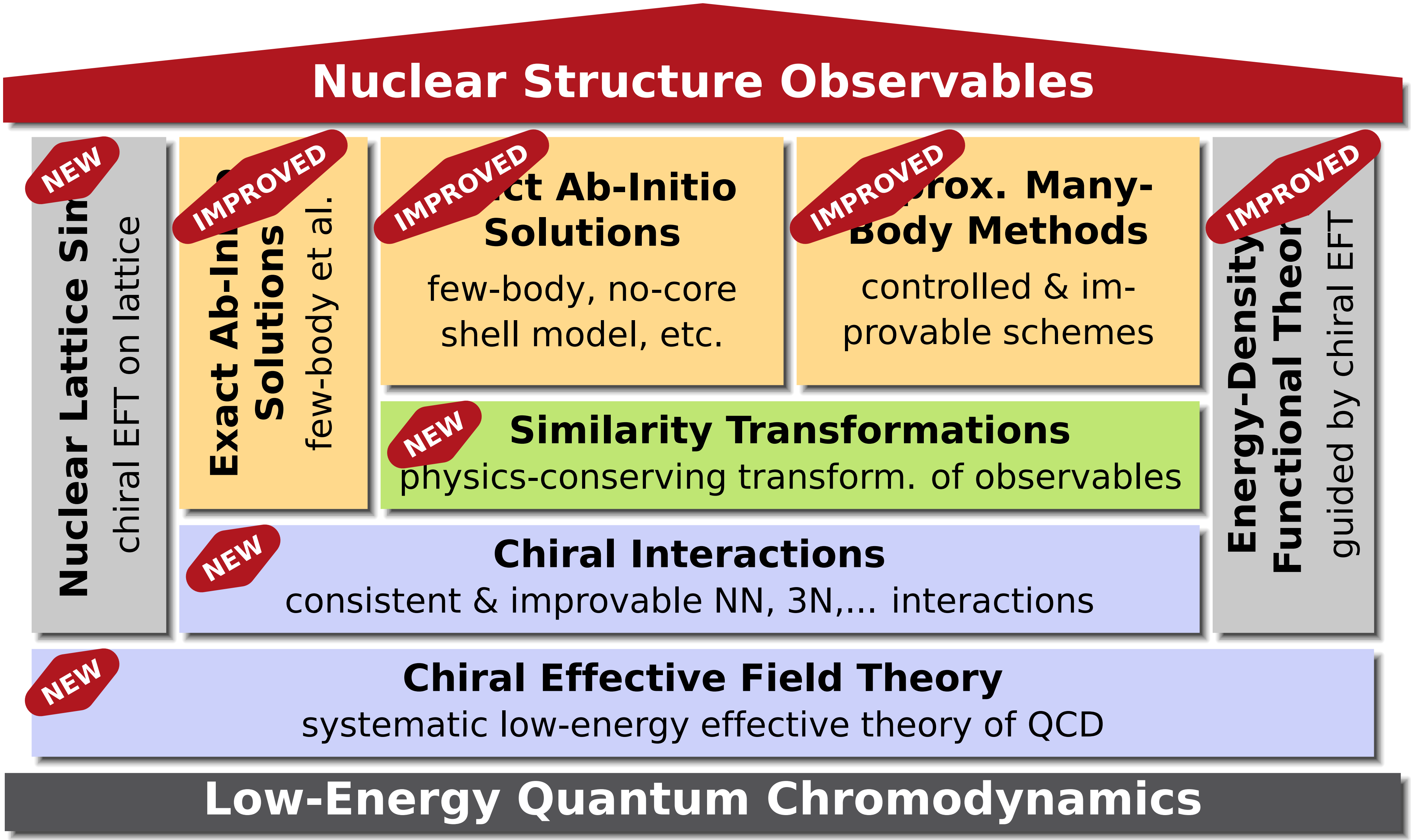
Quantum Chromodynamics

chiral effective field theory and lattice simulations access low-energy QCD and nuclear interactions

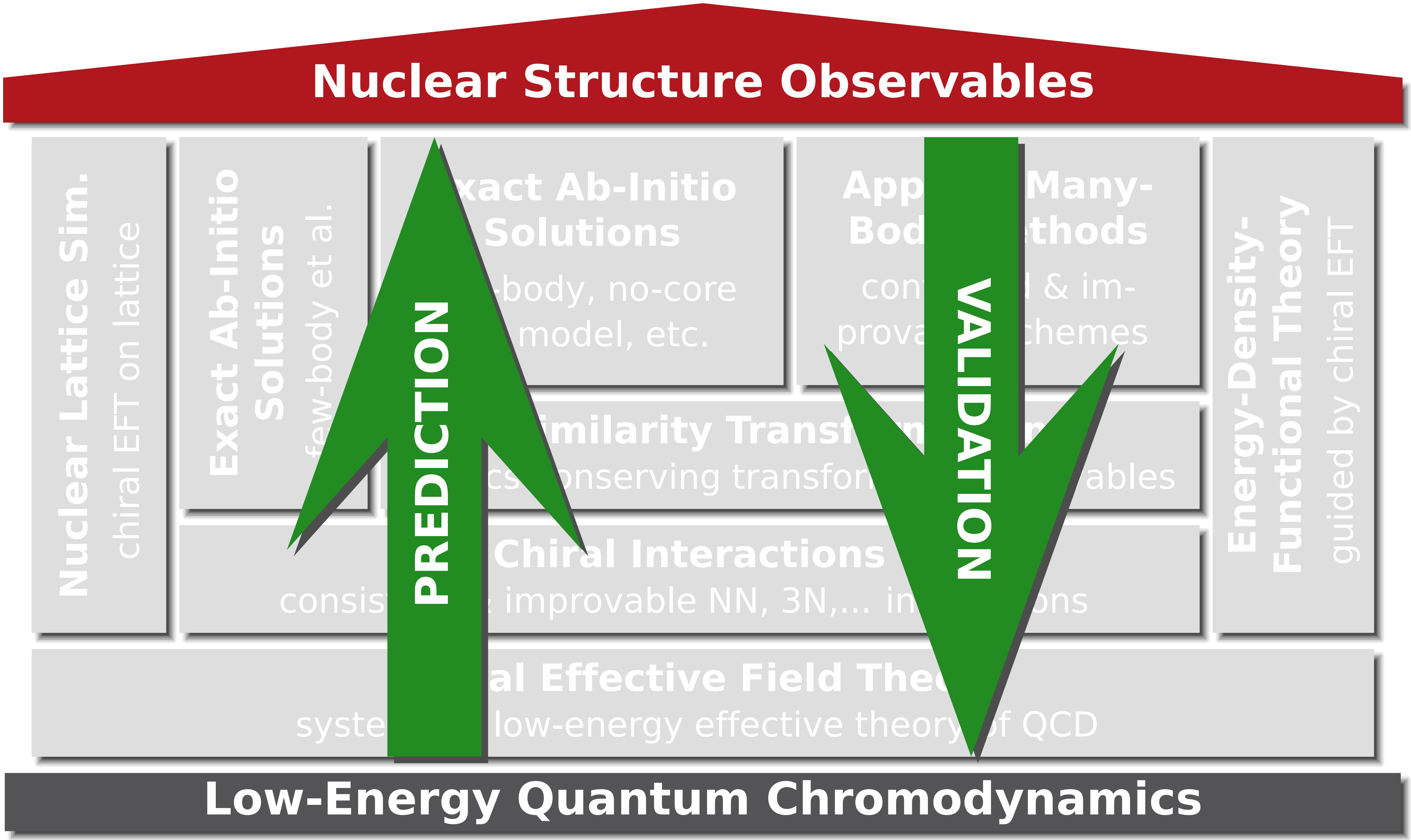
Nuclear Many-Body Theory

novel theoretical and computational methods allow for ab initio description of many more nuclei

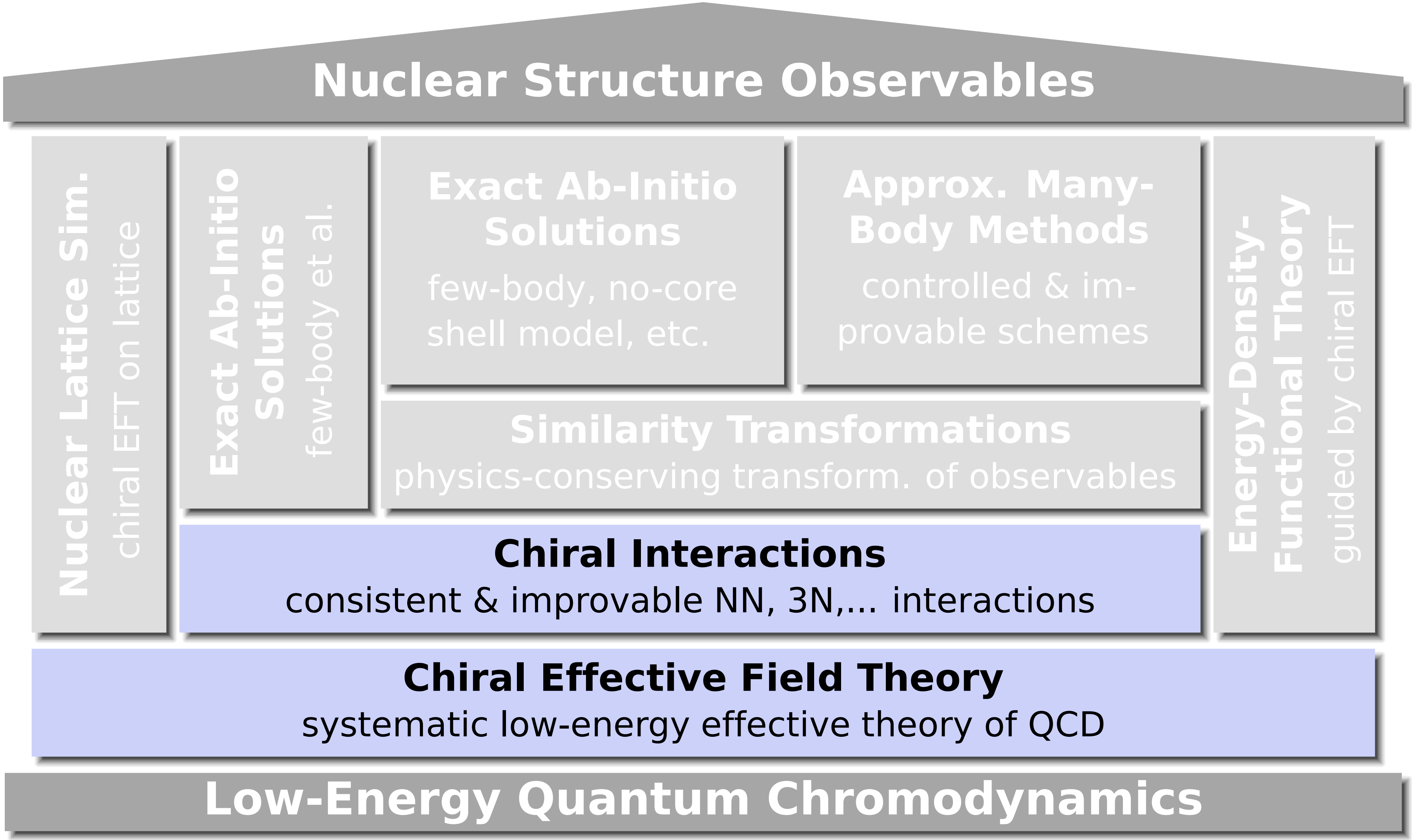
Ab Initio Nuclear Structure



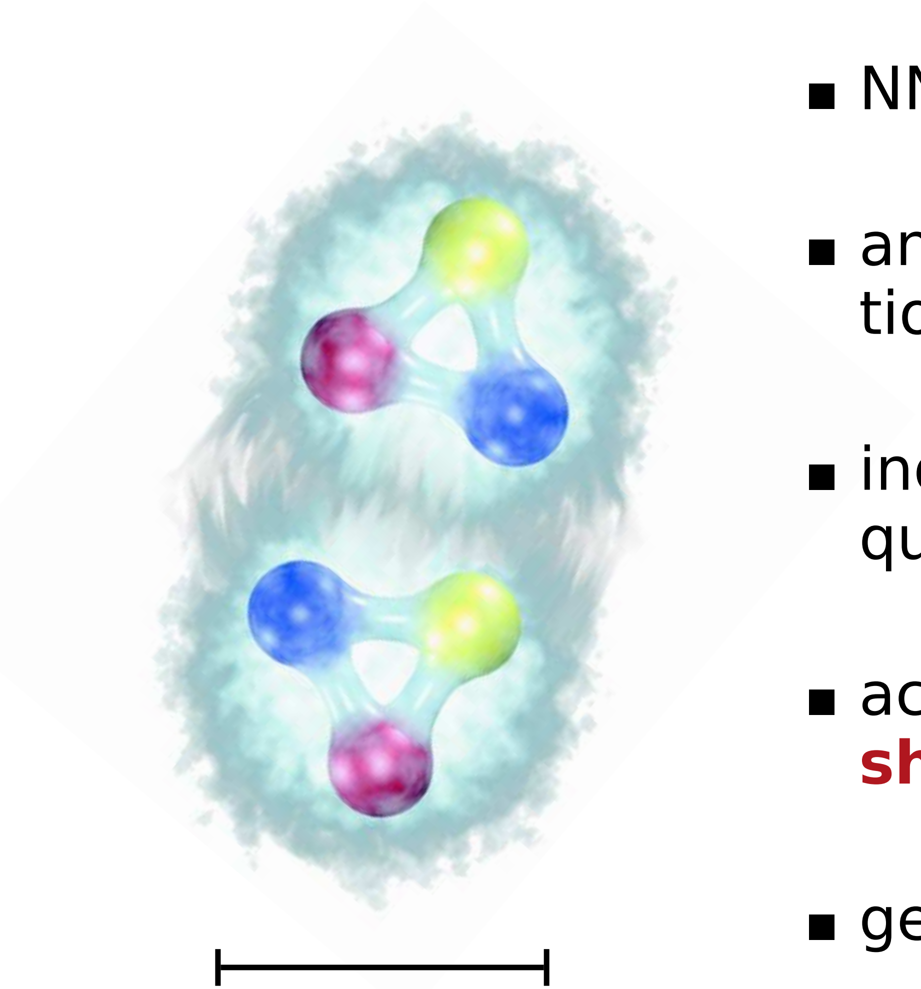
Ab Initio Nuclear Structure



Ab Initio Nuclear Structure



Nature of the Nuclear Interaction

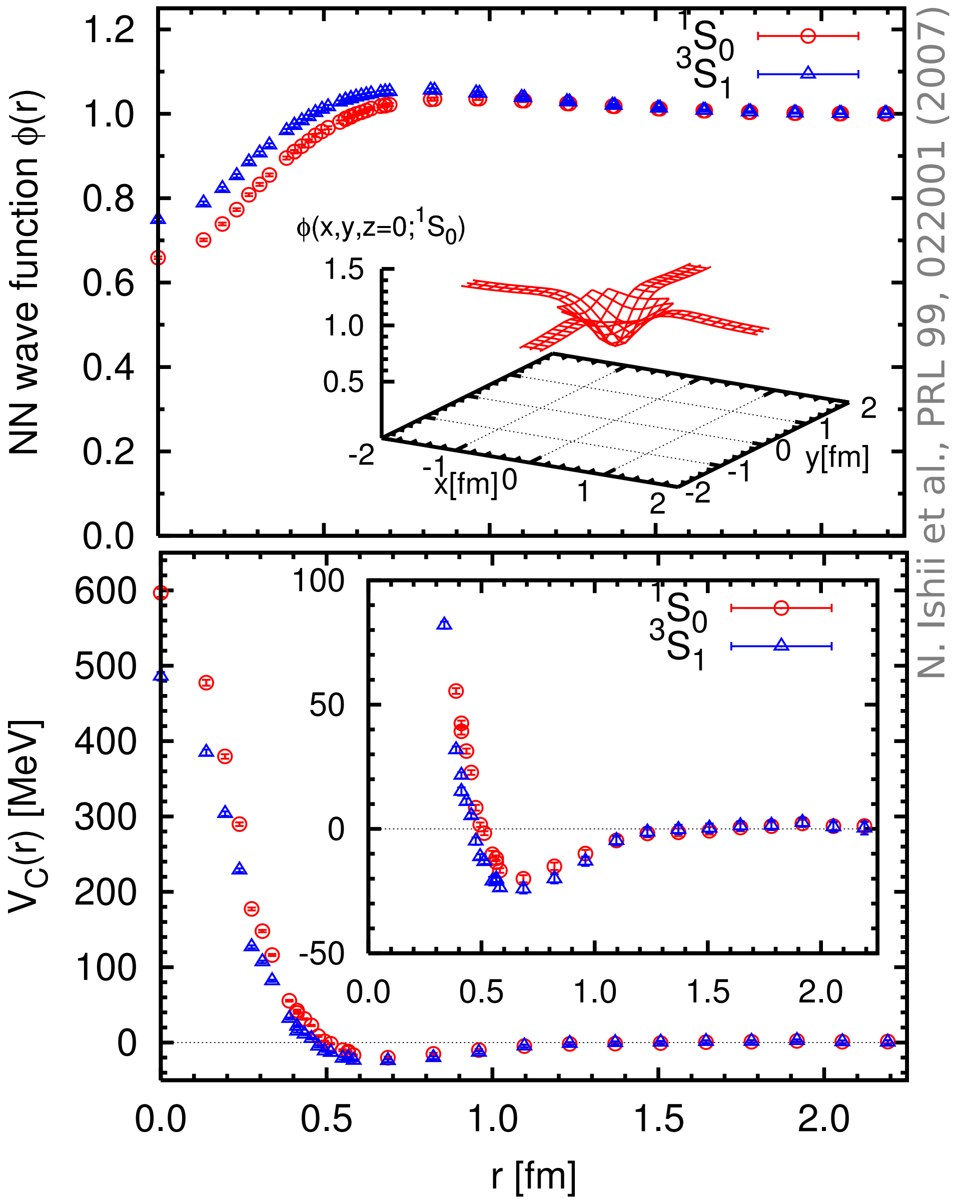


$\sim 1.6\text{fm}$

$\rho_0^{-1/3} = 1.8\text{fm}$

- NN-interaction is **not fundamental**
- analogous to **van der Waals** interaction between neutral atoms
- induced via mutual **polarization** of quark & gluon distributions
- acts only if the nucleons overlap, i.e. at **short ranges**
- genuine **3N-interaction** is important

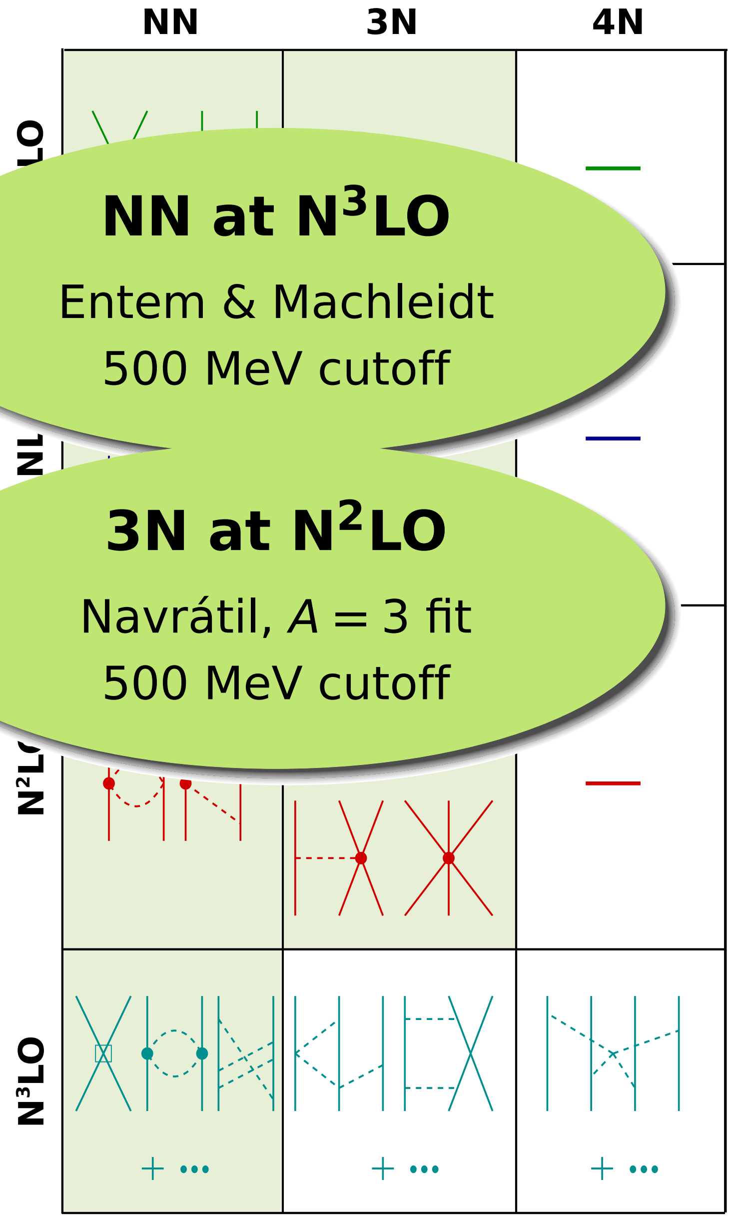
Nuclear Interaction from Lattice QCD



- first steps towards construction of a nuclear interaction through **lattice QCD simulations**
- compute relative **two-nucleon wavefunction** on the lattice
- invert Schrödinger equation to obtain **local 'effective' two-nucleon potential**
- schematic results so far (un-physical quark masses, S-wave interactions only,...)

Nuclear Interactions from Chiral EFT

- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- long-range **pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment (NN, πN,...)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at N^3LO
  - explicit inclusion of Δ-resonance
  - formal issues: power counting, renormalization, cutoff choice,...



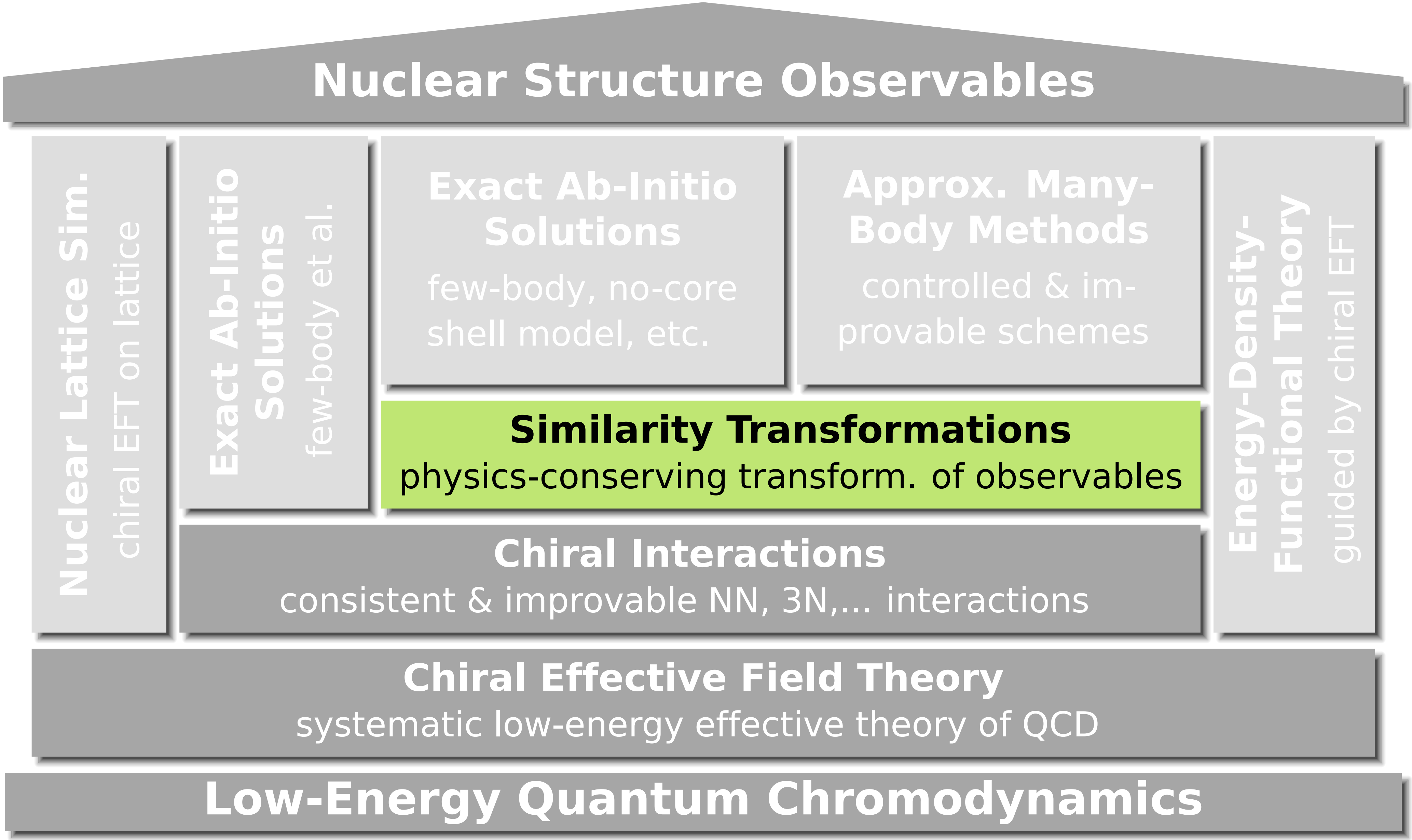
NN at N^3LO

Entem & Machleidt
500 MeV cutoff

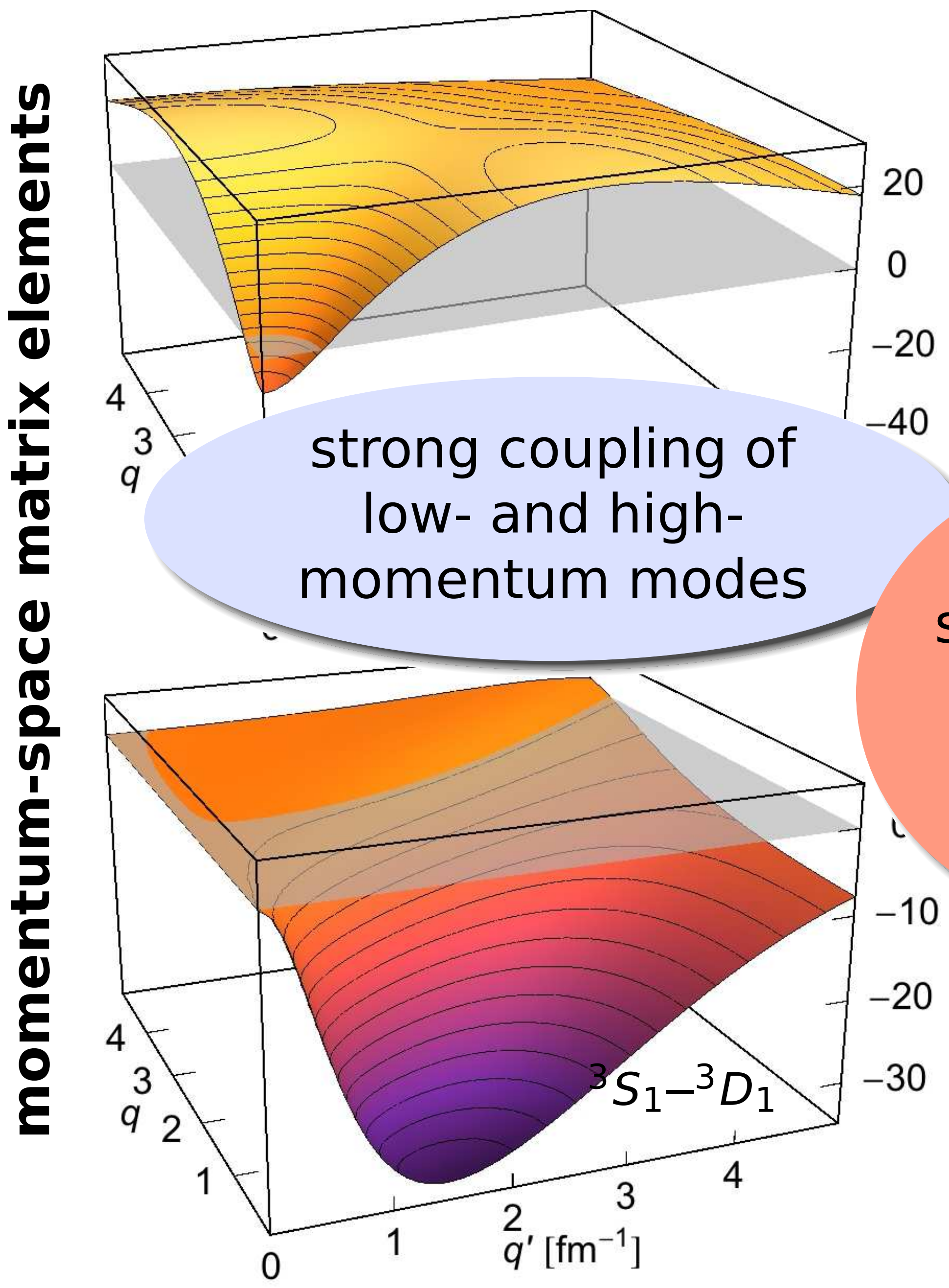
3N at N^2LO

Navrátil, $A = 3$ fit
500 MeV cutoff

Ab Initio Nuclear Structure



Why Similarity Transformations?



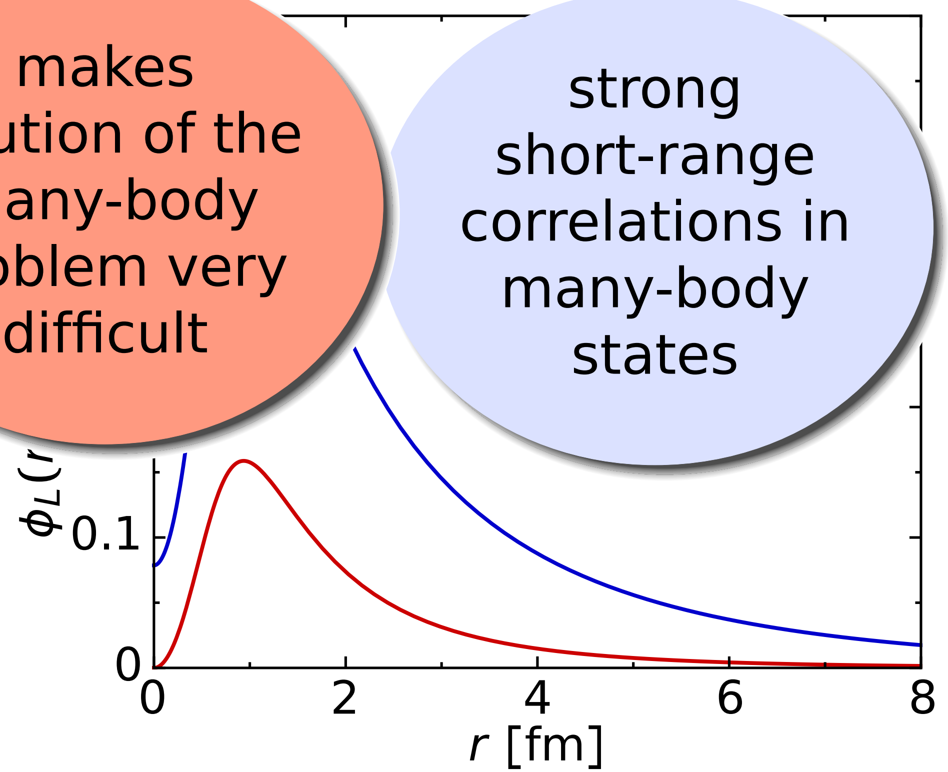
strong coupling of low- and high-momentum modes

makes solution of the many-body problem very difficult

Argonne V18

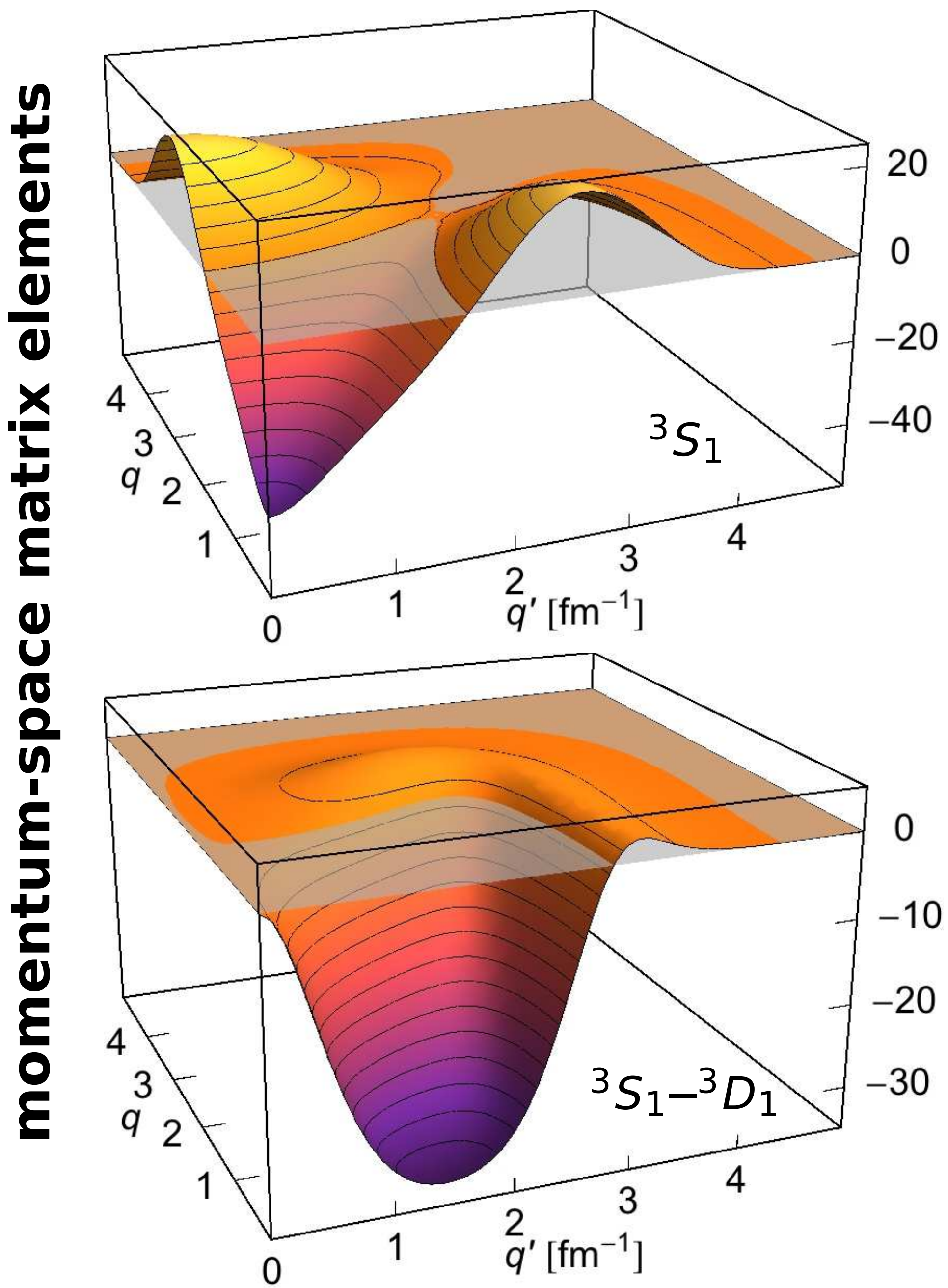
$J^\pi = 1^+, T = 0$

deuteron wave-function



strong short-range correlations in many-body states

Why Similarity Transformations?

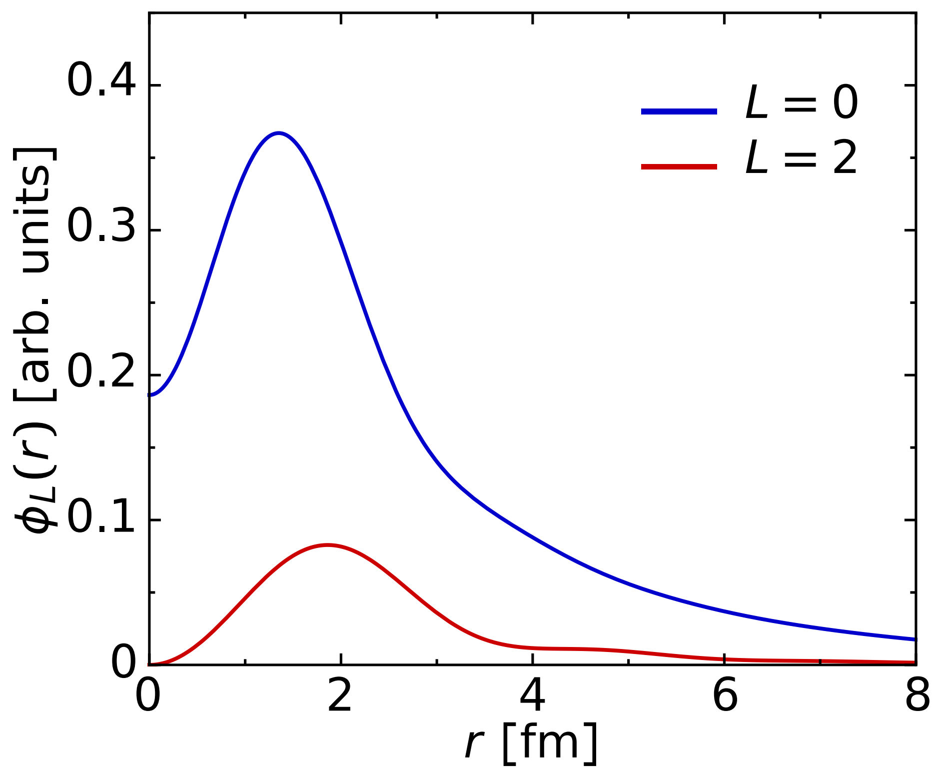


chiral N^{3}LO

Entem & Machleidt, 500 MeV

$J^\pi = 1^+, T = 0$

deuteron wave-function



Similarity Renormalization Group

continuous transformation driving
Hamiltonian to band-diagonal form
with respect to a chosen basis

simplicity and flexibility are great advantages of the SRG approach

solve SRG evolution equations using two- & three-body matrix representation

- **unitary transformation** of Hami

$$\widetilde{H}_\alpha = U_\alpha^\dagger H U_\alpha$$

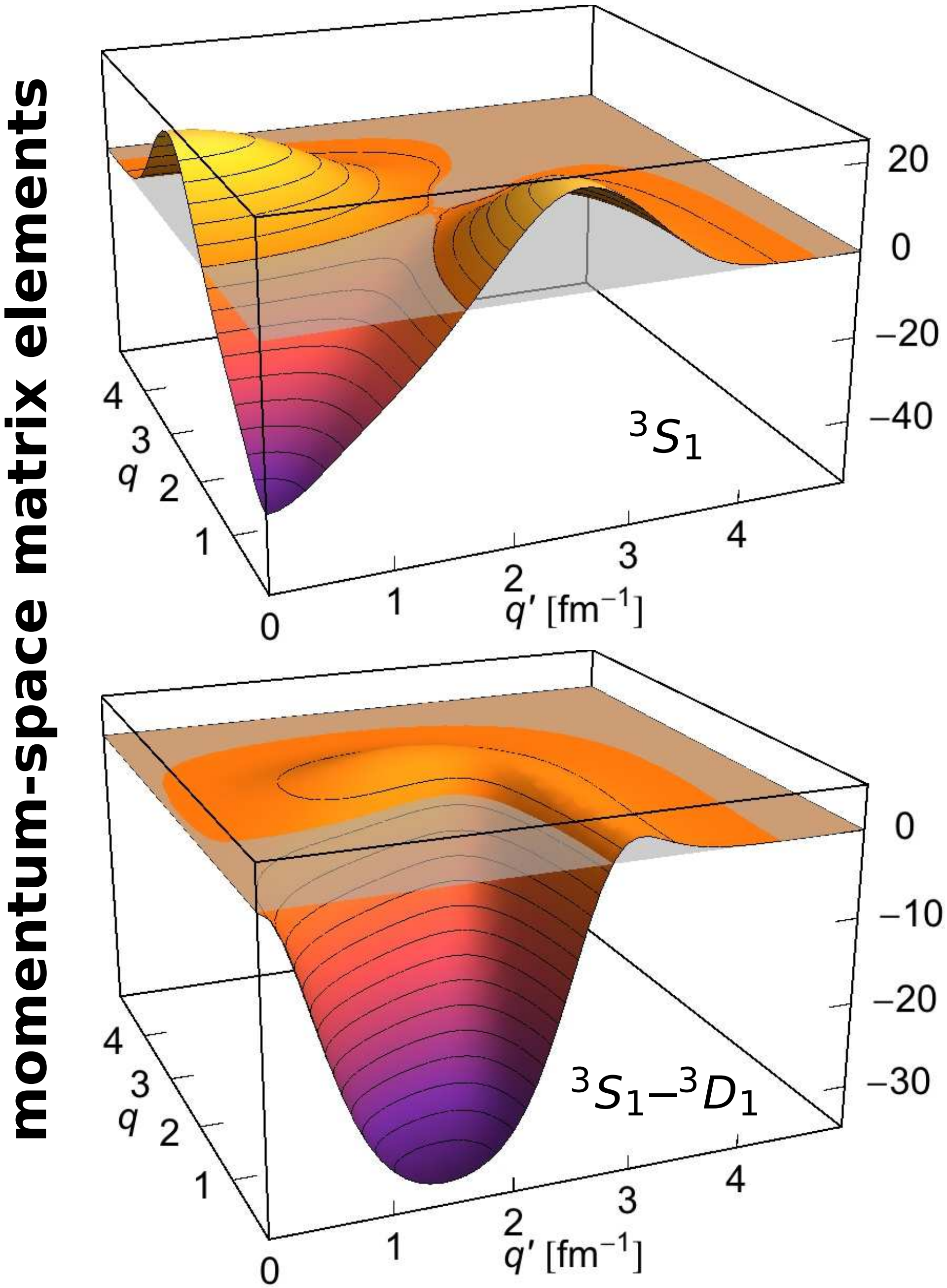
- **evolution equations** for $\widetilde{H}_\alpha$ and U

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha]$$

- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta_\alpha = (2\mu)^2 [T_{int}, \widetilde{H}_\alpha]$$

SRG Evolution in Two-Body Space

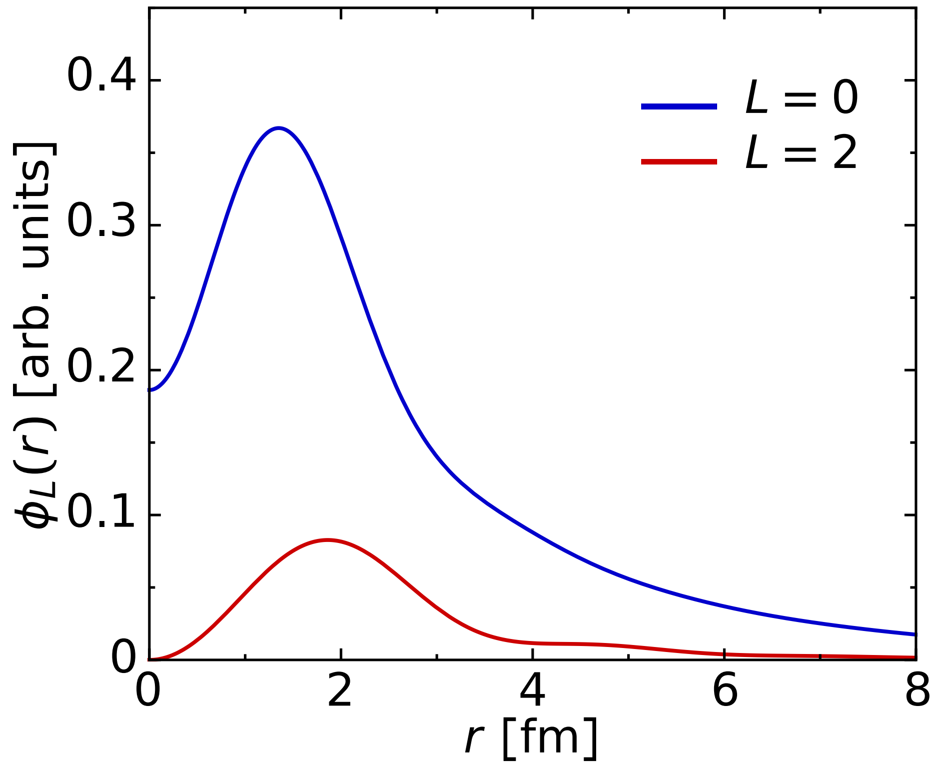


$\alpha = 0.000\,\mathrm{fm}^4$

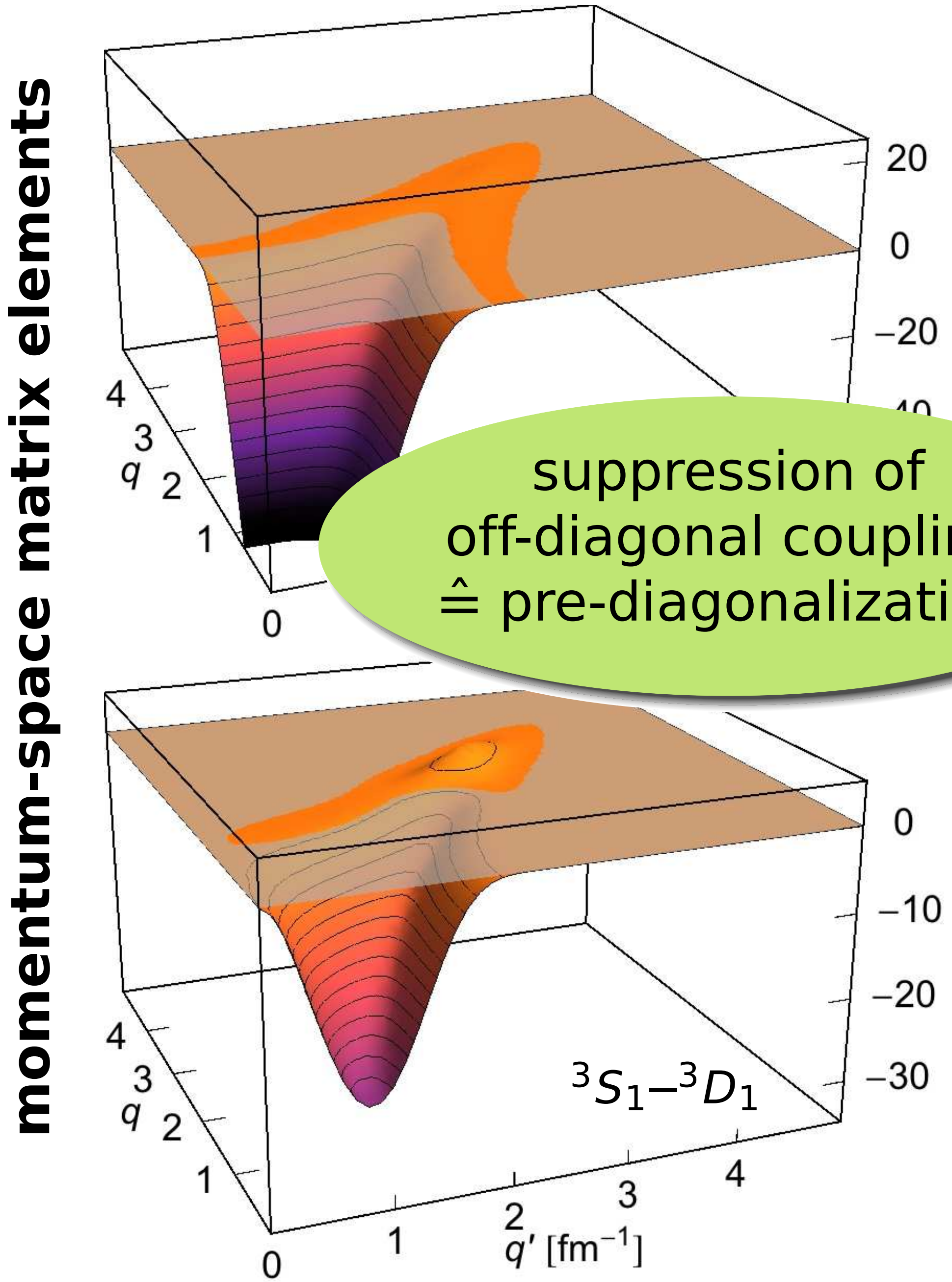
$\Lambda = \infty\,\mathrm{fm}^{-1}$

$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG Evolution in Two-Body Space

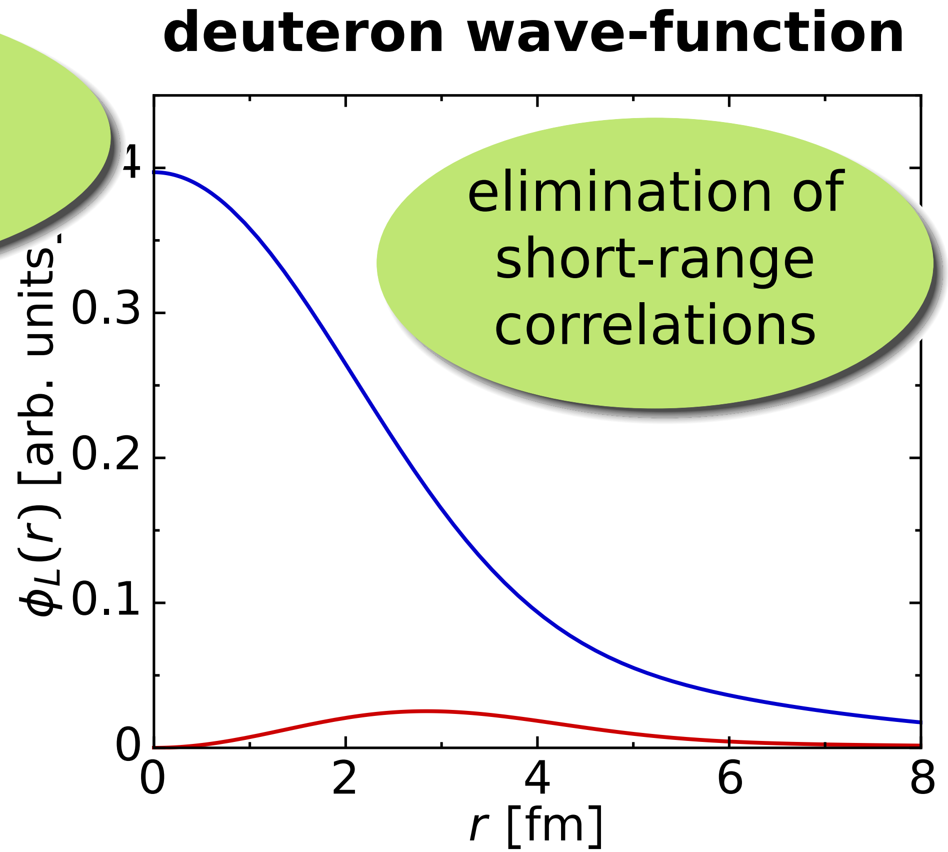


$\alpha = 0.320\,\text{fm}^4$

$\Lambda = 1.33\,\text{fm}^{-1}$

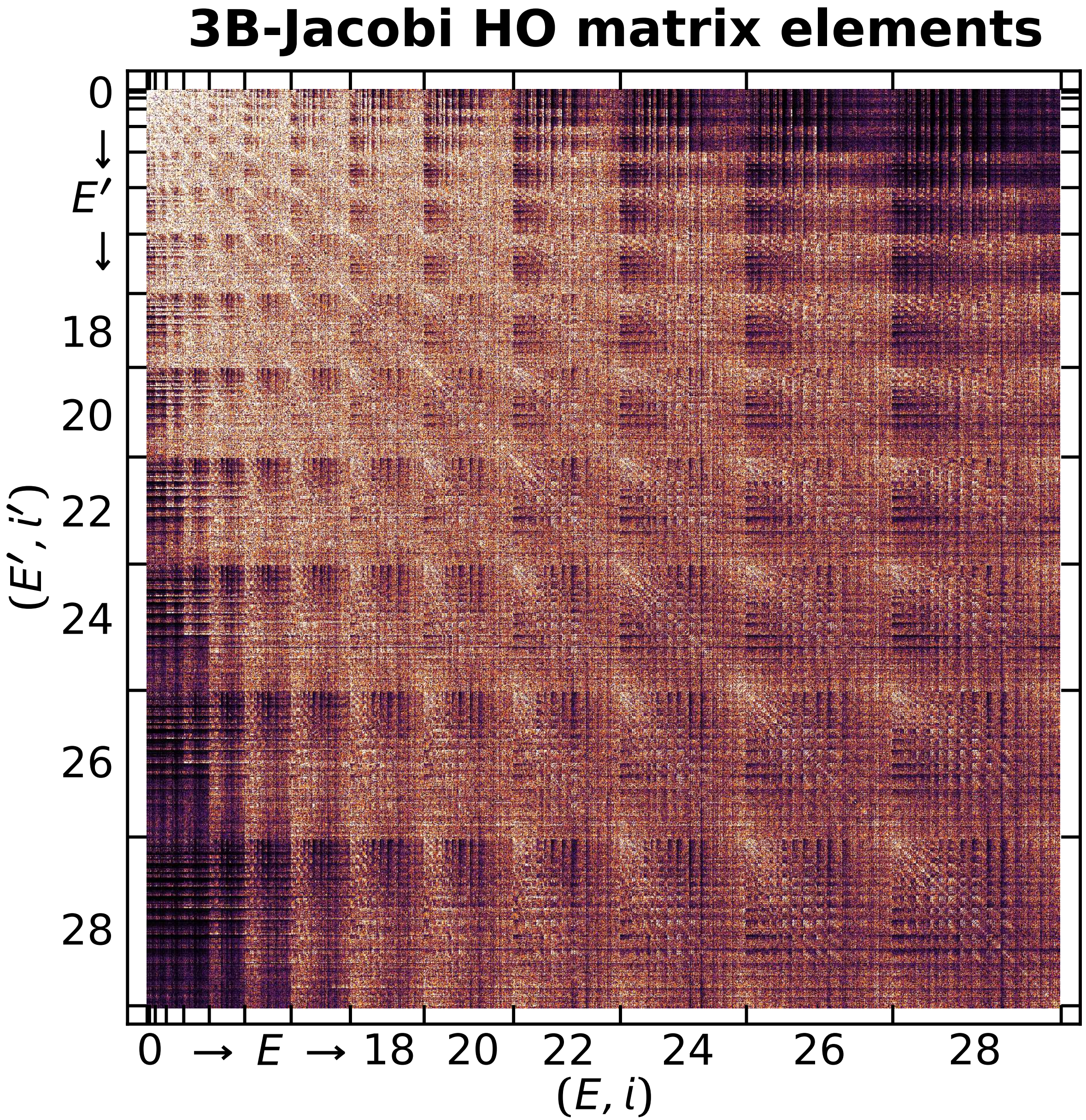
$J^\pi = 1^+, T = 0$

suspression of off-diagonal coupling ≙ pre-diagonalization



elimination of short-range correlations

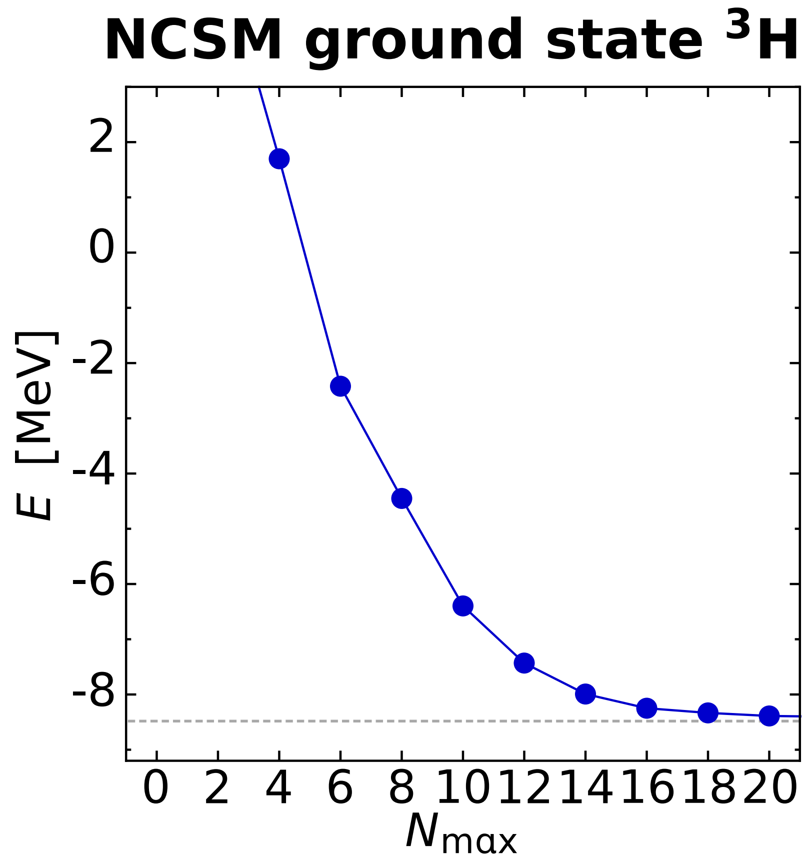
SRG Evolution in Three-Body Space



$\alpha = 0.000\,\text{fm}^4$

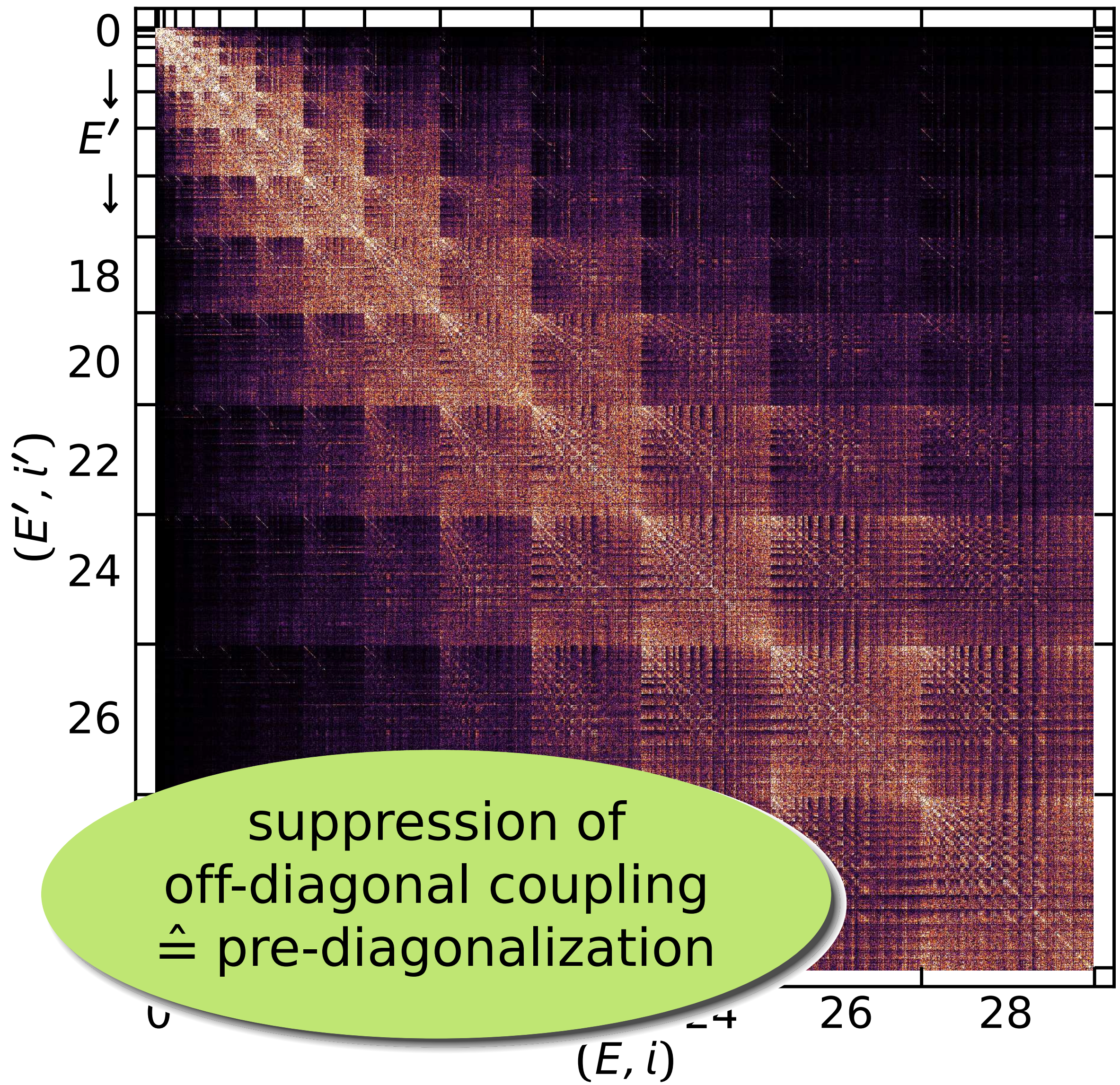
$\Lambda = \infty\,\text{fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\text{MeV}$



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



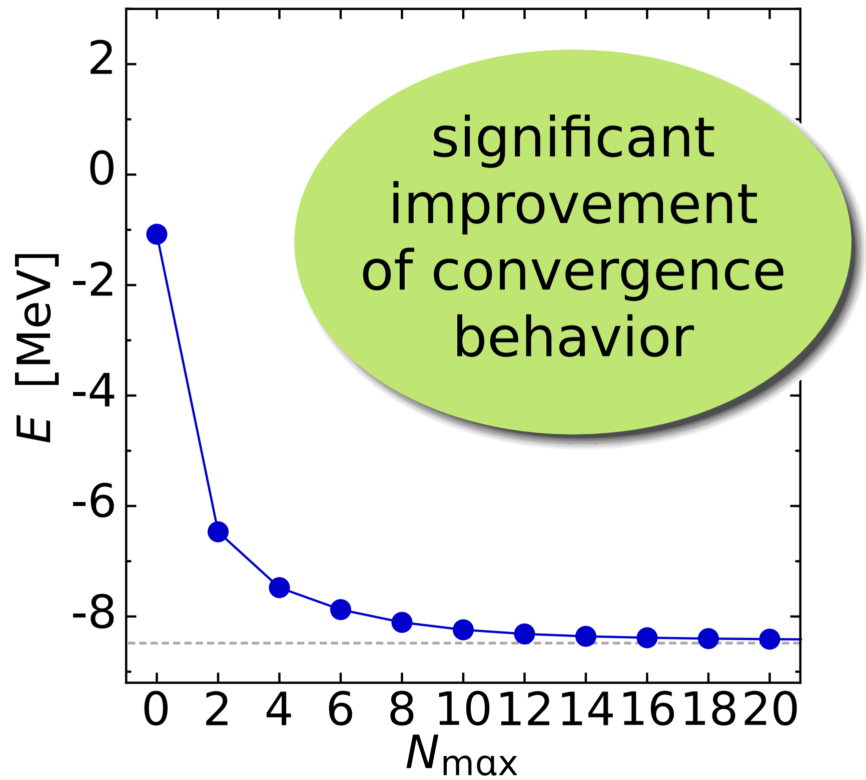
suppression of
off-diagonal coupling
≙ pre-diagonalization

$\alpha = 0.320\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

Calculations in *A*-Body Space

- evolution **induces *n*-body contributions** $\widetilde{H}_{\alpha}^{[n]}$ to Hamiltonian

$$\widetilde{H}_{\alpha} = \widetilde{H}_{\alpha}^{[1]} + \widetilde{H}_{\alpha}^{[2]} + \widetilde{H}_{\alpha}^{[3]} + \widetilde{H}_{\alpha}^{[4]} + \ldots$$

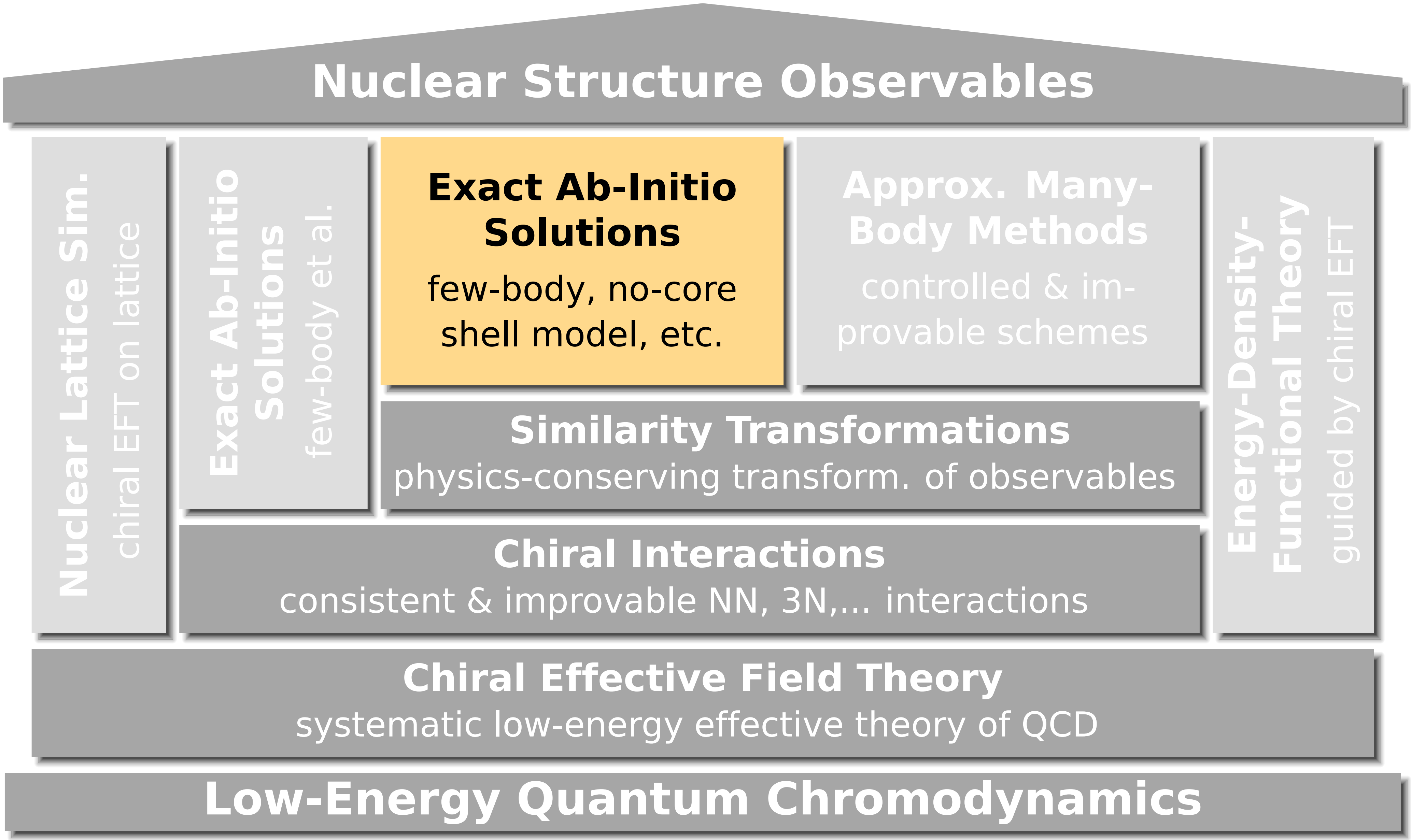
- truncation of cluster series inevitable — formally destroys unitarity and invariance of energy eigenvalues (independence of α)

Three SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Ham[...] keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3[...] and all three-body terms

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

Ab Initio Nuclear Structure



No-Core Shell Model — Basics

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\max}\hbar\Omega$

- numerical solution of **matrix eigenvalue problem** for the intrinsic Hamiltonian H within truncated model space

$$\mathrm{H}|\Psi\rangle = E|\Psi\rangle \quad \rightarrow \quad \begin{pmatrix} & \vdots & \\ \dots & \langle\Phi_\nu|\mathrm{H}|\Phi_\mu\rangle & \dots \\ & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ C_\mu \\ \vdots \end{pmatrix} = E \begin{pmatrix} \vdots \\ C_\nu \\ \vdots \end{pmatrix}$$

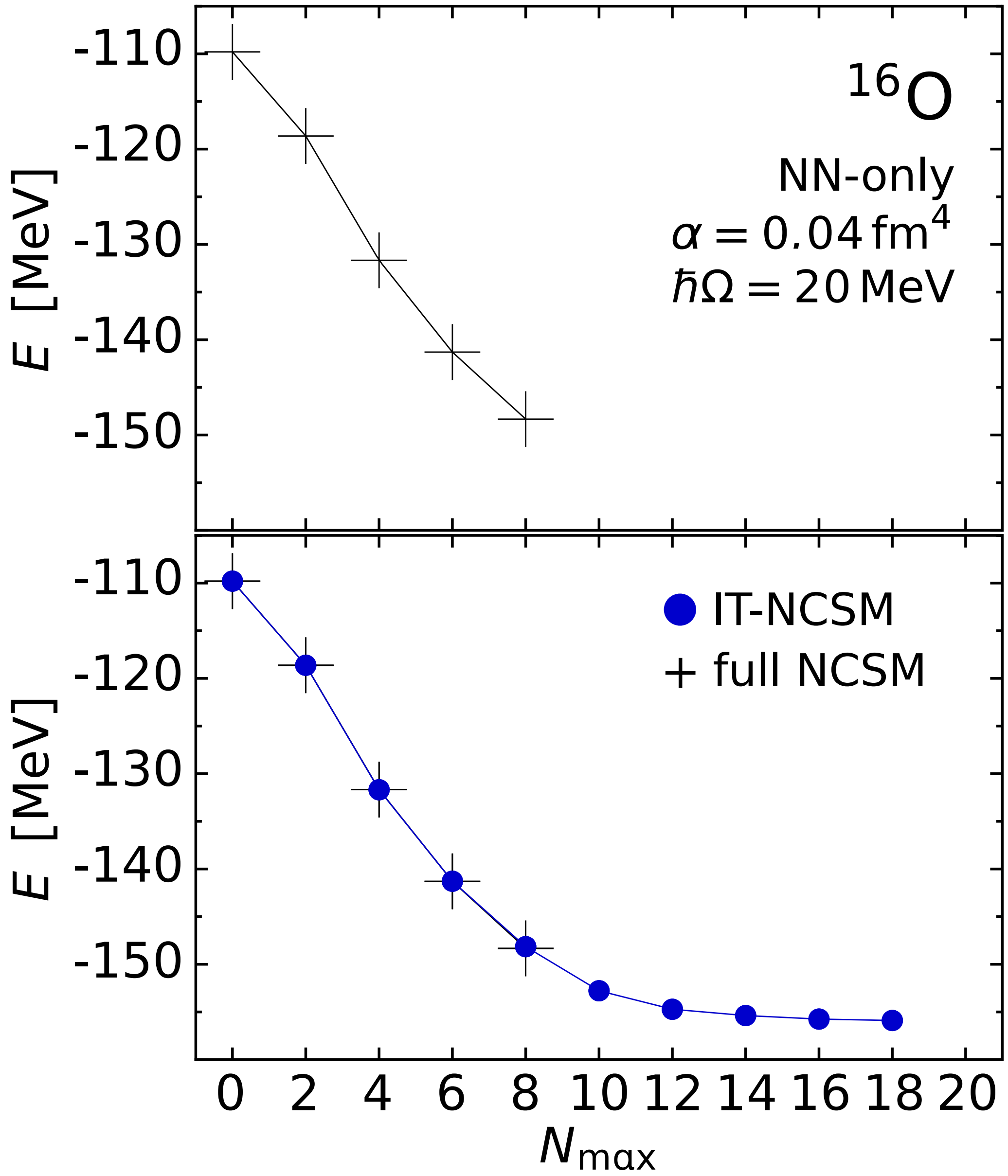
- model spaces of **up to 10^9 basis states** are used routinely

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for ^{16}O getting very difficult (basis dimension > 10^{10})

Importance Truncation

reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



Importance Truncation: General Idea

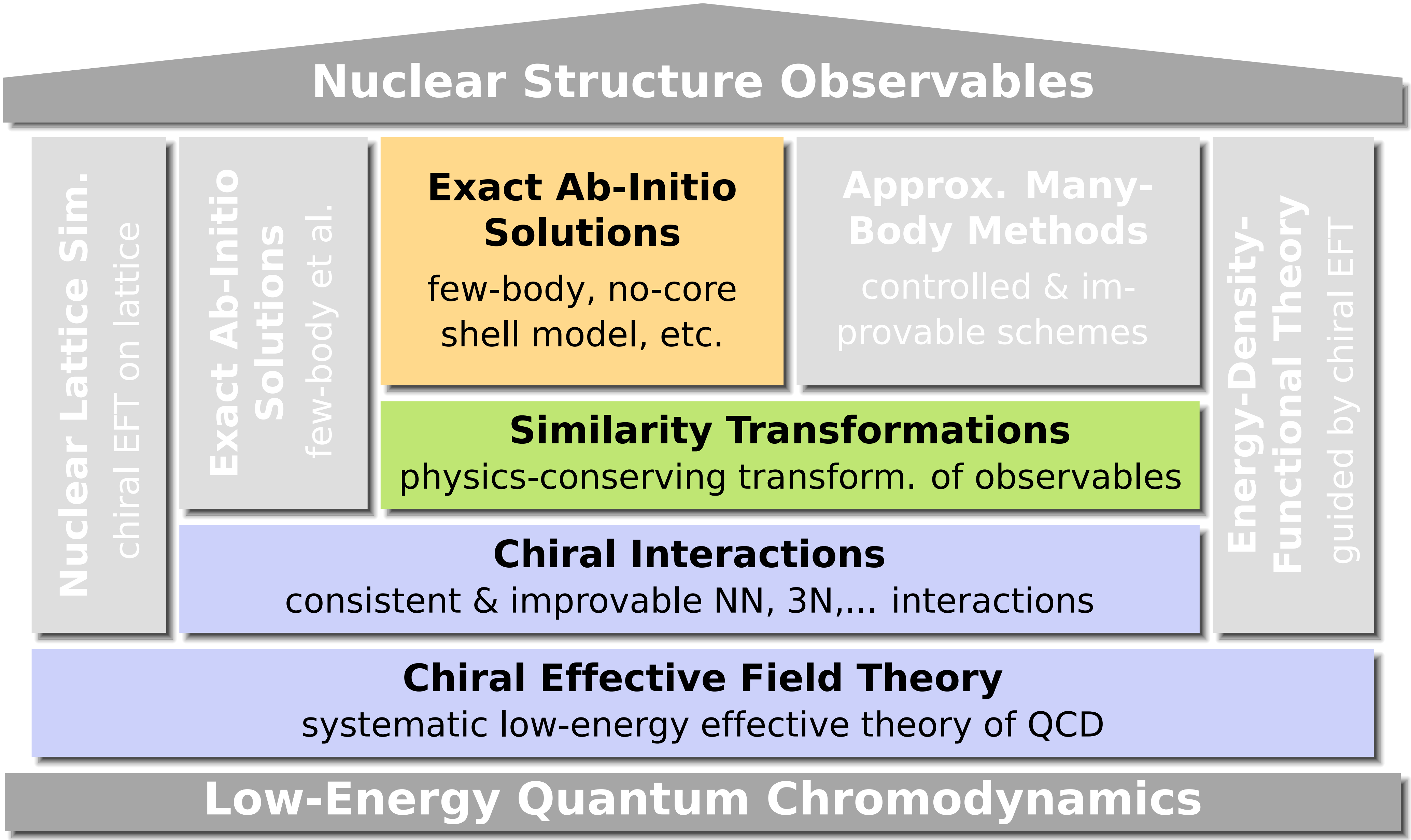
- given an initial approximation $\left|\Psi_{\text{ref}}^{(m)}\right\rangle$ for the **target states**
- **measure the importance** of individual basis state $\left|\Phi_\nu\right\rangle$ via first-order multiconfigurational perturbation theory

$$\kappa_\nu^{(m)} = -\frac{\left\langle \Phi_\nu \middle| \mathrm{H} \middle| \Psi_{\text{ref}}^{(m)} \right\rangle}{\Delta\epsilon_\nu}$$

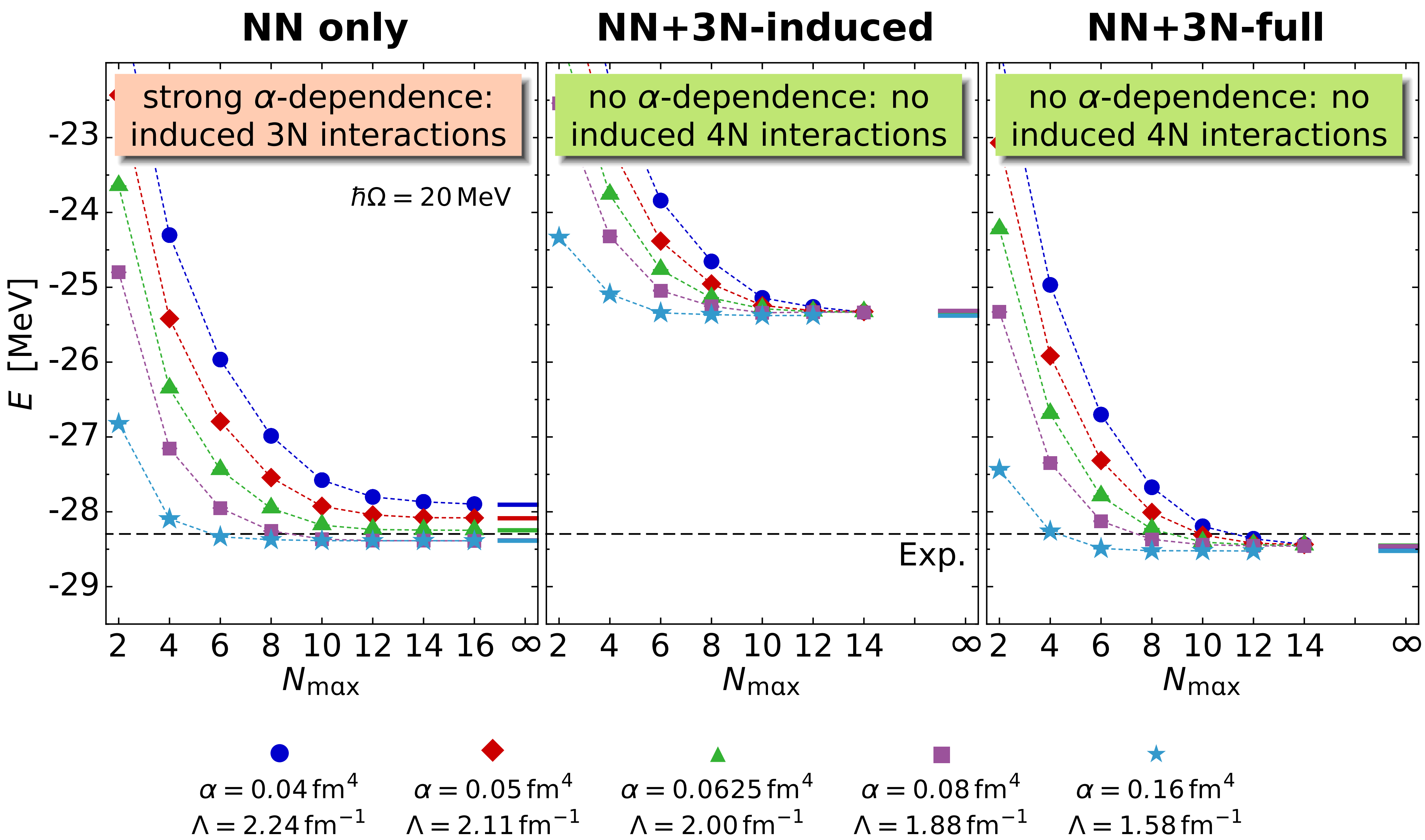
- construct **importance truncated space** spanned by basis states with $|\kappa_\nu^{(m)}| \geq \kappa_{\text{min}}$ and solve eigenvalue problem
- **sequential scheme**: constru… next N_{max} using previous eigen…
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contributions from discarded basis states

for $\kappa_{\text{min}} \to 0$ the full NCSM model space and thus the **exact solution is recovered**

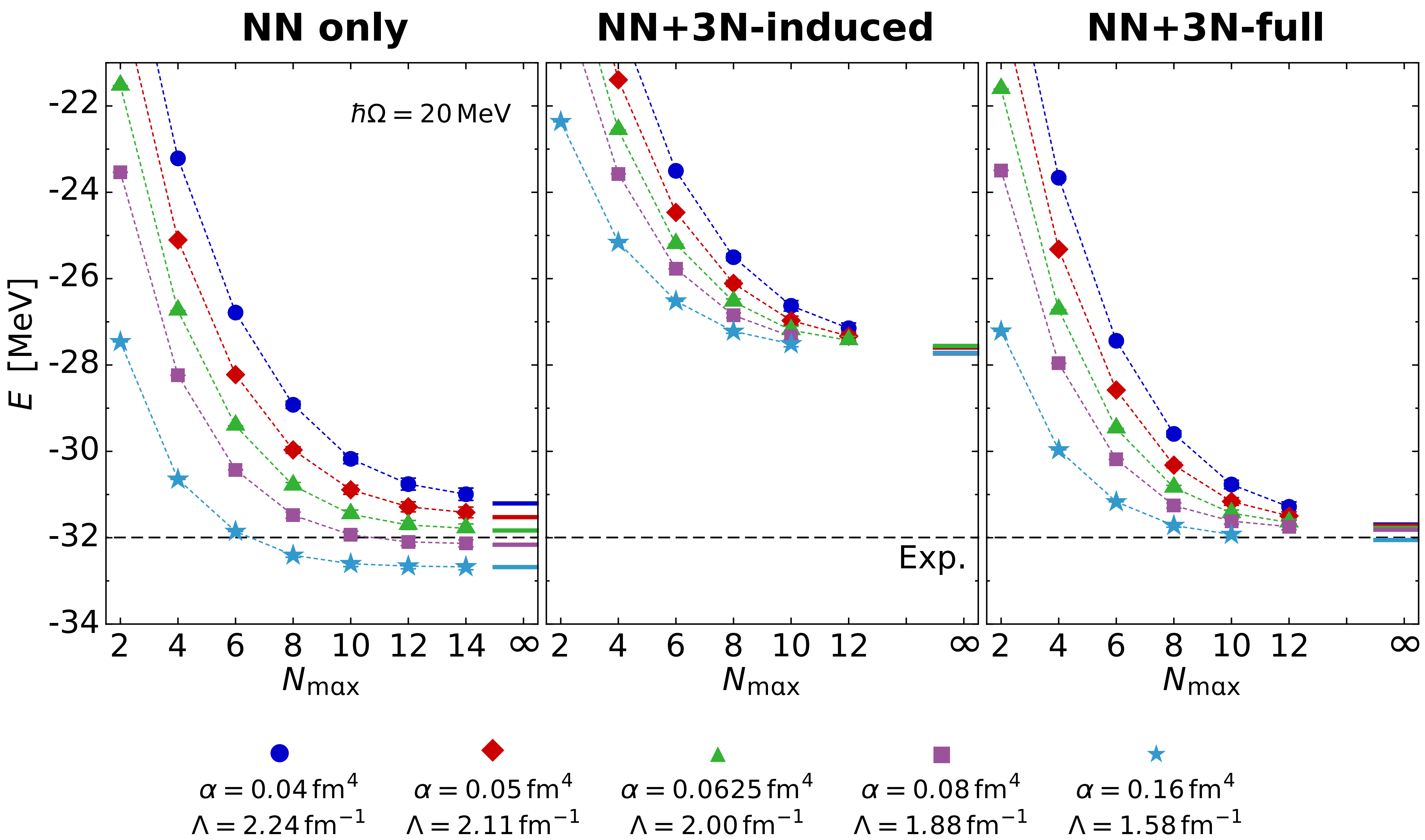
Ab Initio Nuclear Structure



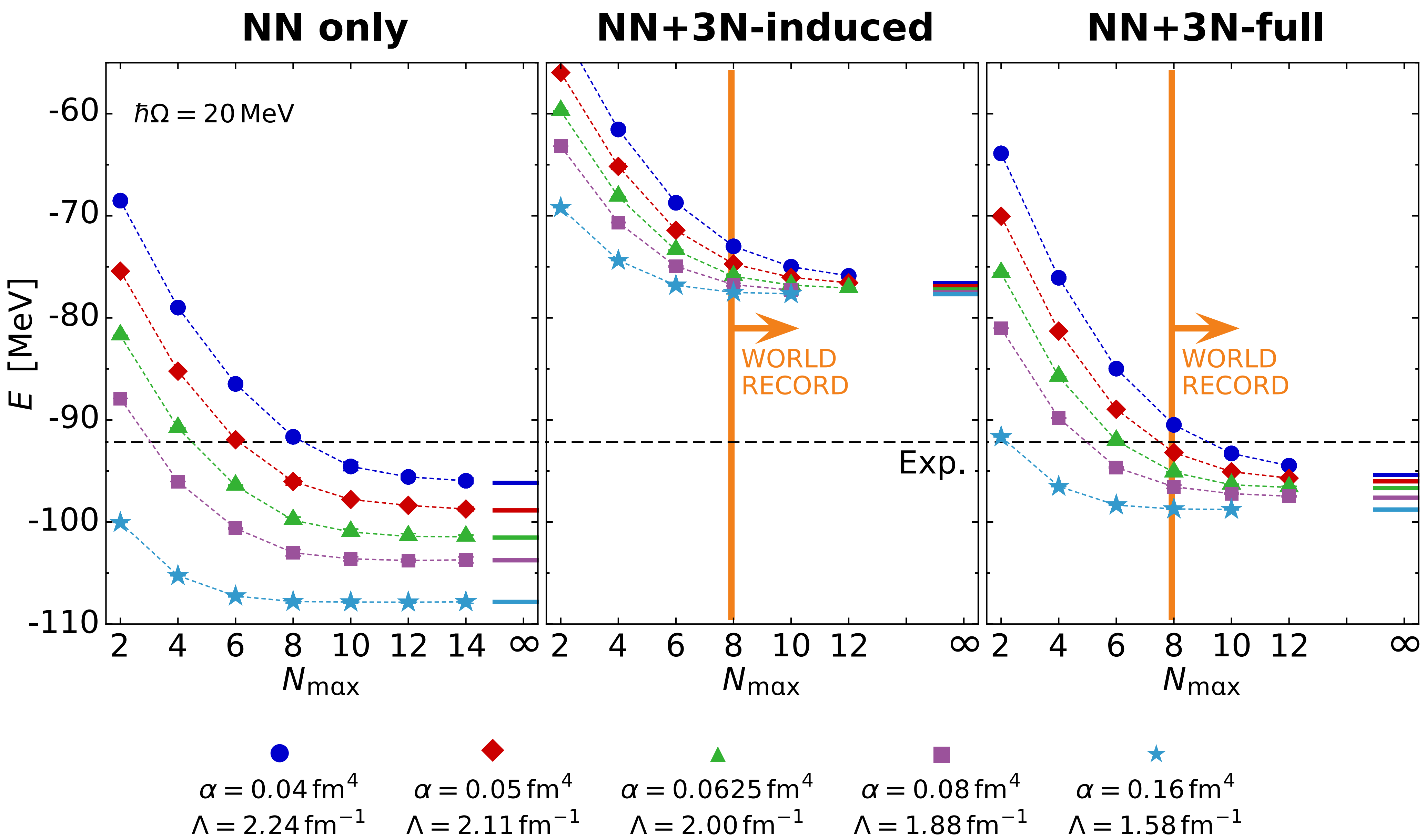
^{4}He: Ground-State Energies



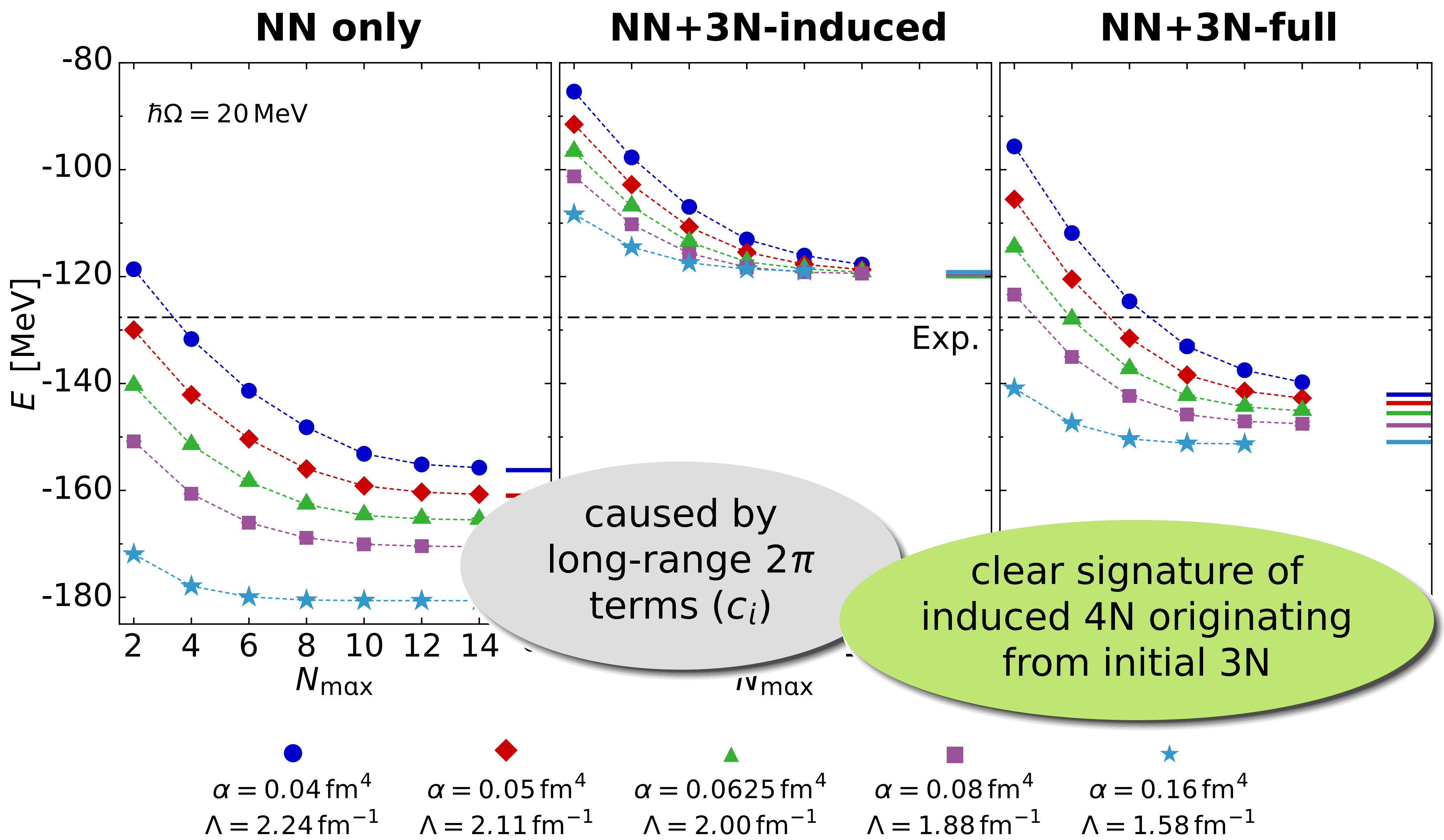
^{6}Li: Ground-State Energies



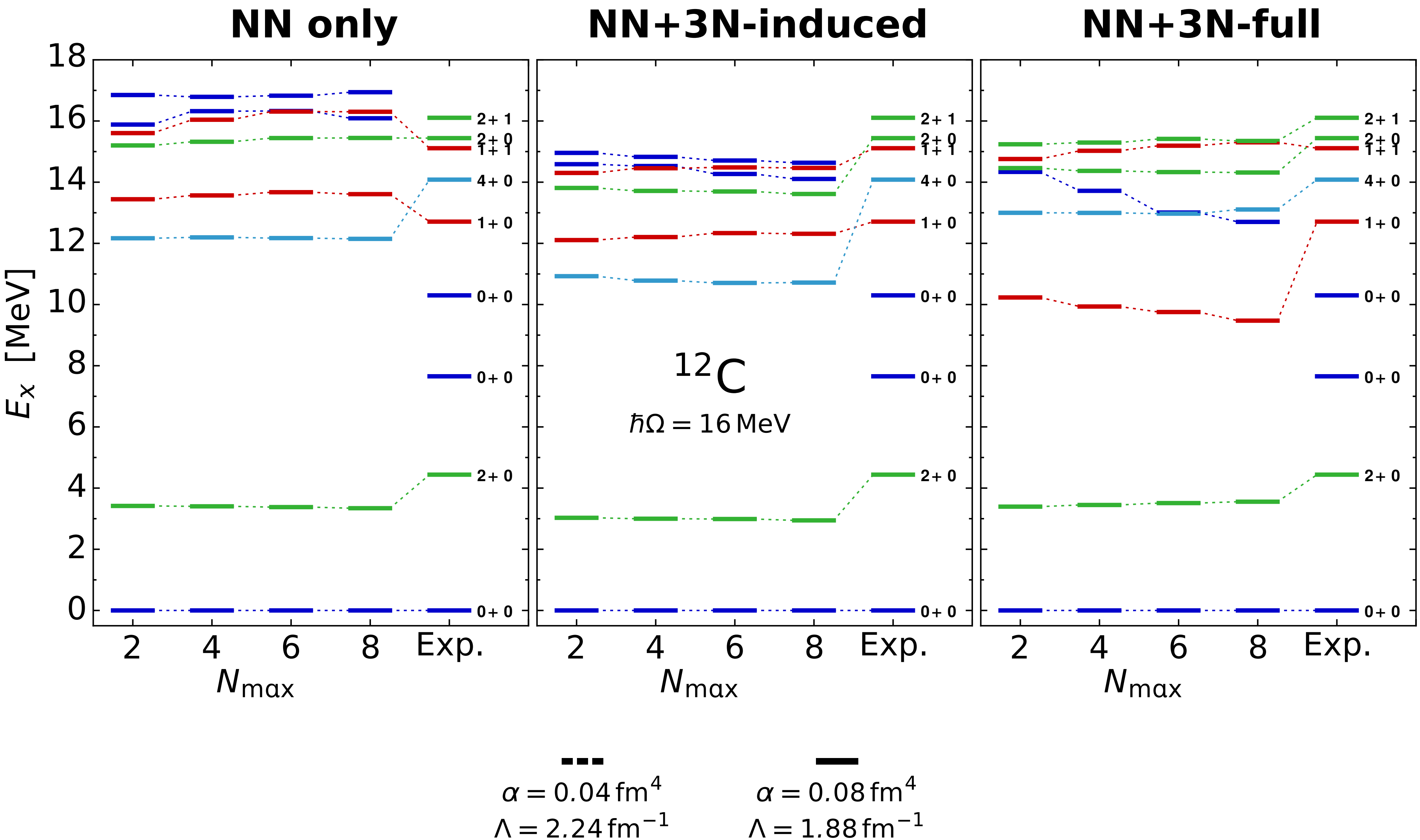
^{12}C: Ground-State Energies



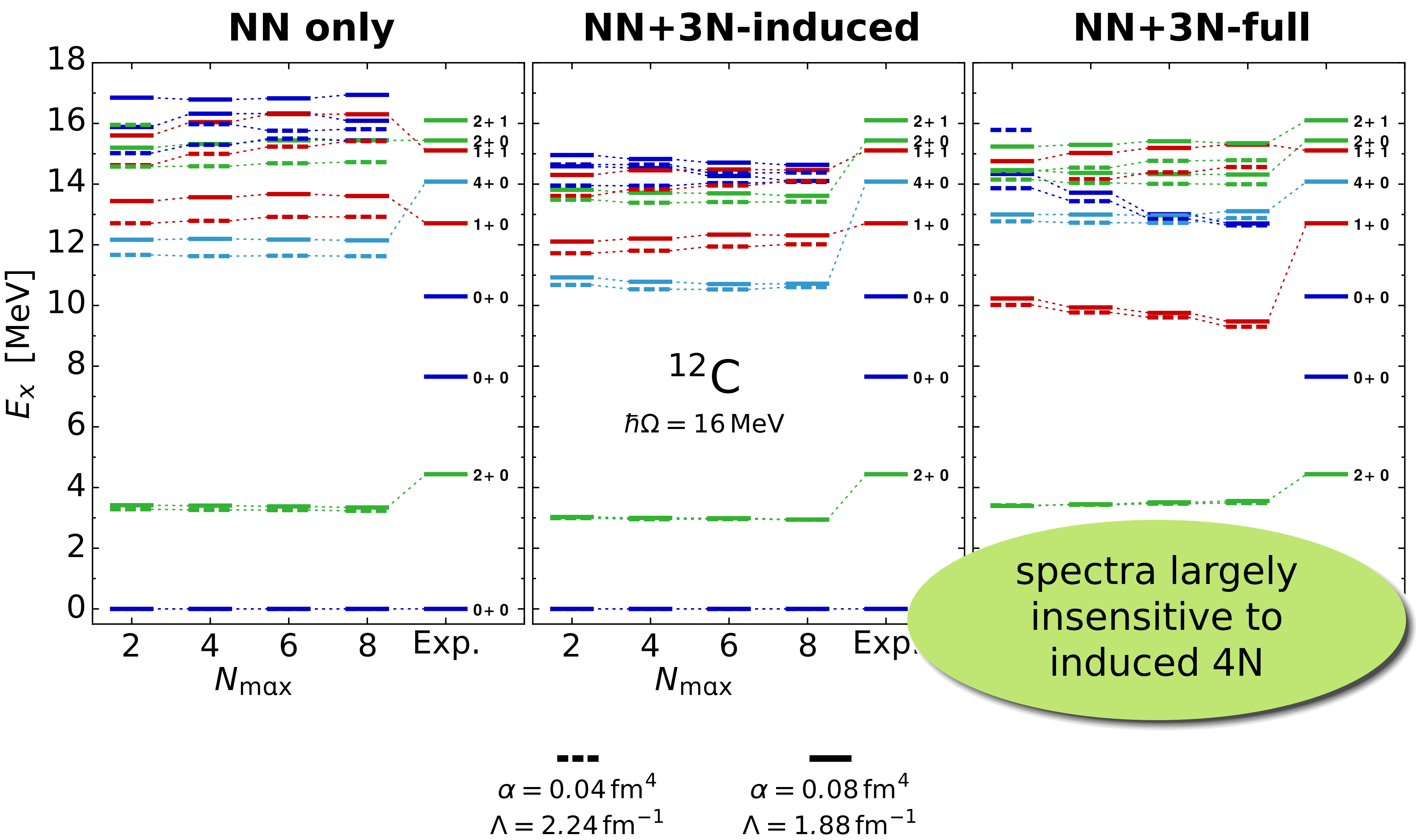
^{16}O: Ground-State Energies



Spectroscopy of ^{12}C



Spectroscopy of ^{12}C



spectra largely insensitive to induced 4N

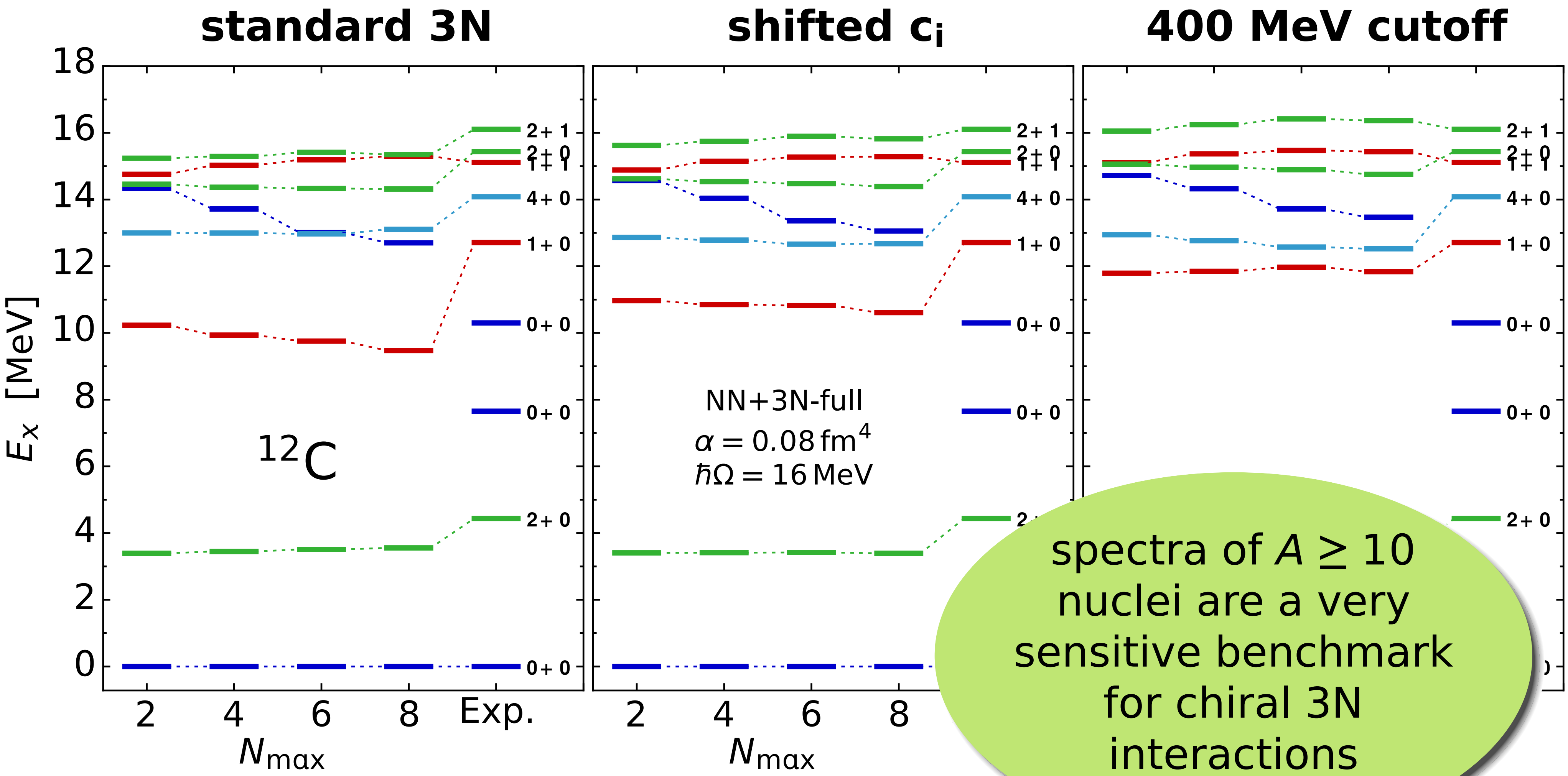
The Bottom Line...

- beyond the lightest nuclei, **SRG-induced 4N contributions** affect the absolute energies (but not the excitation energies)
- with the inclusion of the leading 3N interaction we already obtain a **good description** of spectra (and ground states)
- **breakthrough** in computation, transformation and management of 3N matrix-elements

- **next-generation SRG**: can we find new SRG-generators that do not induce as much 4N but still give good convergence?
- **next-generation chiral 3N**: how will N3LO or Δ-full chiral 3N interactions affect the picture?
- **applications**: which experiment-related applications are in reach with the present framework?

Outlook: Sensitivity on Initial 3N

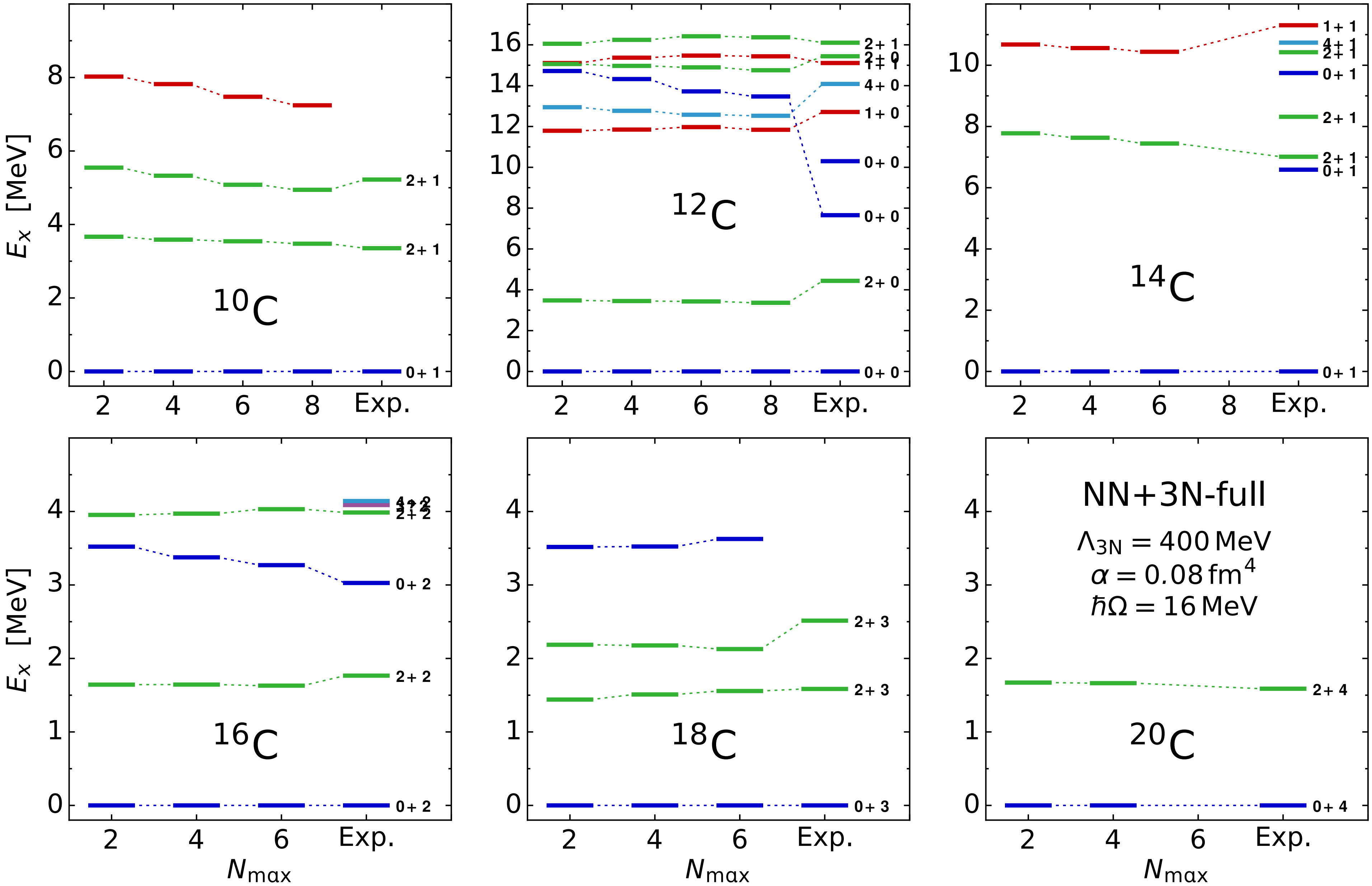
modified 3N interaction* with



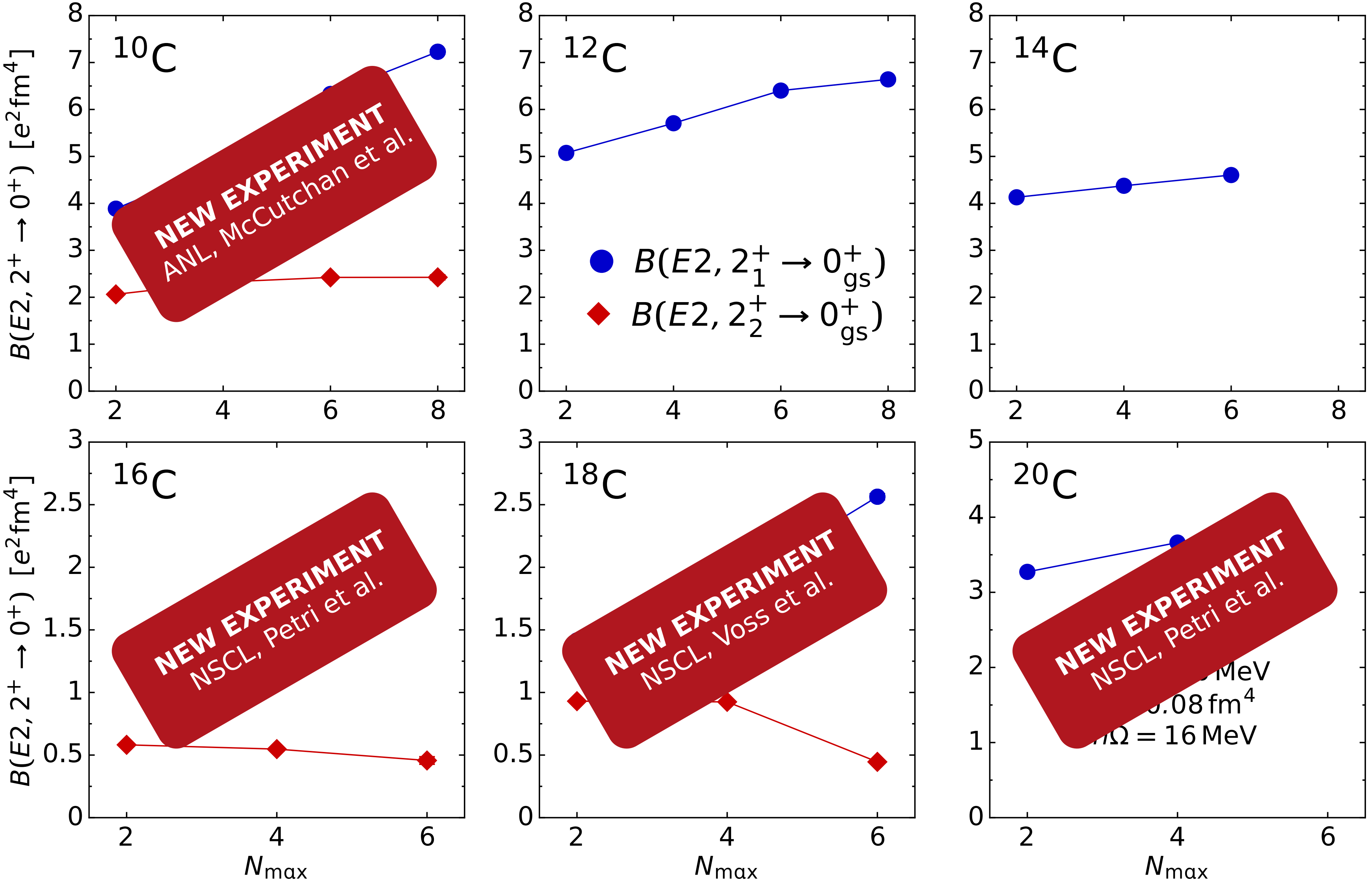
spectra of $A \geq 10$ nuclei are a very sensitive benchmark for chiral 3N interactions

* c_E refit to ^{4}He ground-state energy

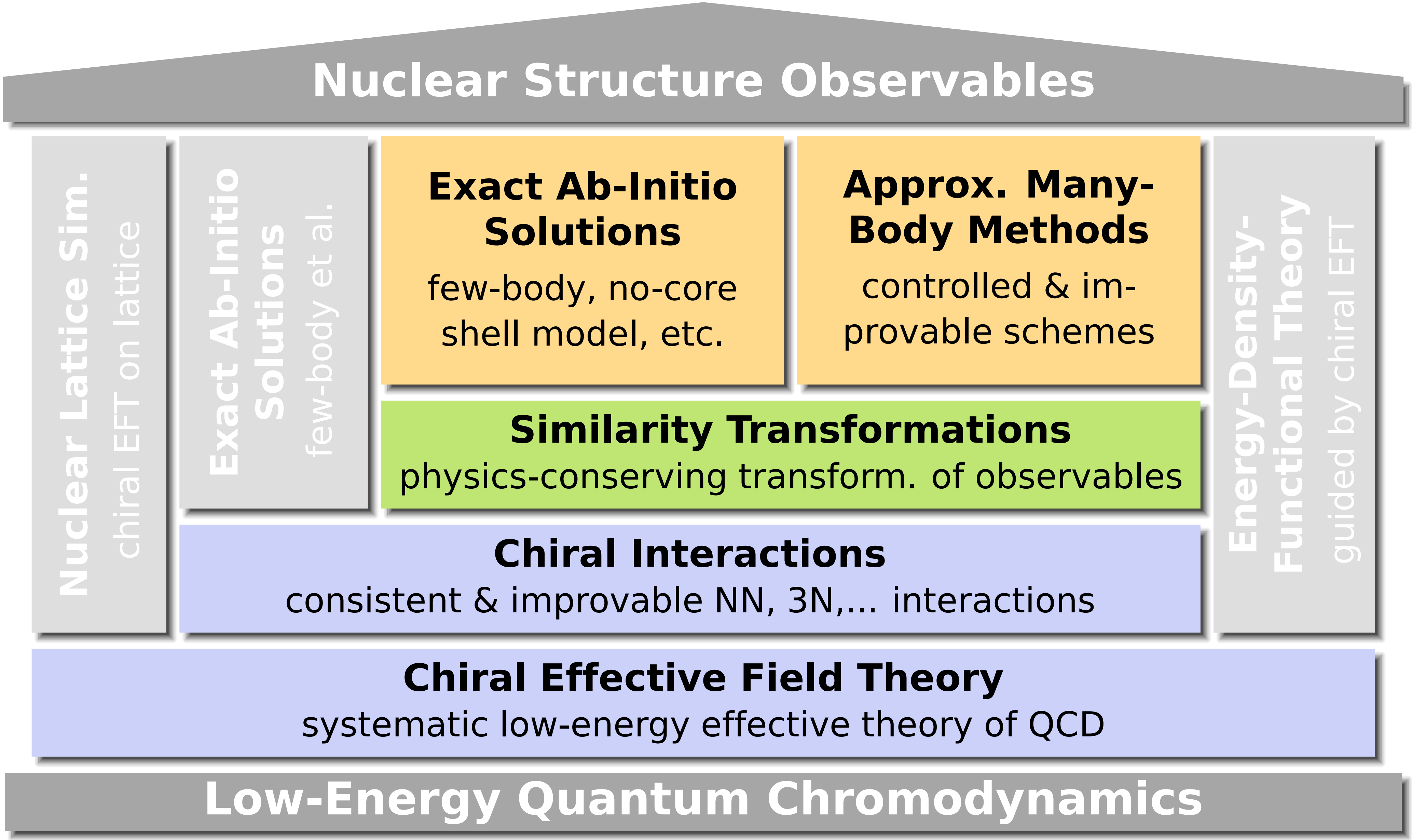
Outlook: Carbon Isotopic Chain



Outlook: Carbon Isotopic Chain



Ab Initio Nuclear Structure



Heavy Nuclei with 3N Interactions

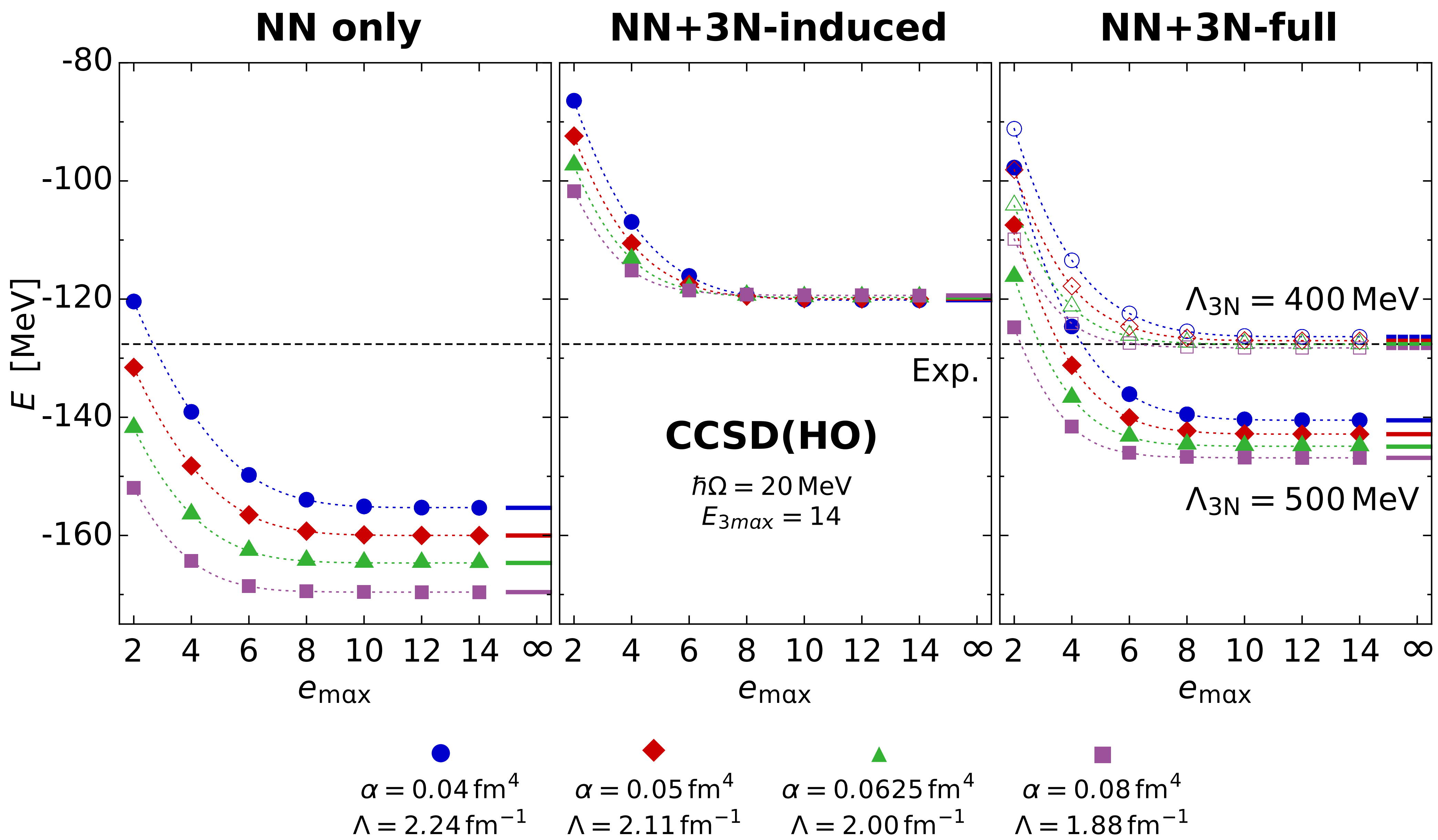
'ab initio' calculations for heavier nuclei require alternative many-body tools and approximate treatment of 3N interactions

- **coupled-cluster method** for ground states of closed-shell nuclei
  - exponential ansatz for many-body states using singles and doubles excitations (CCSD)

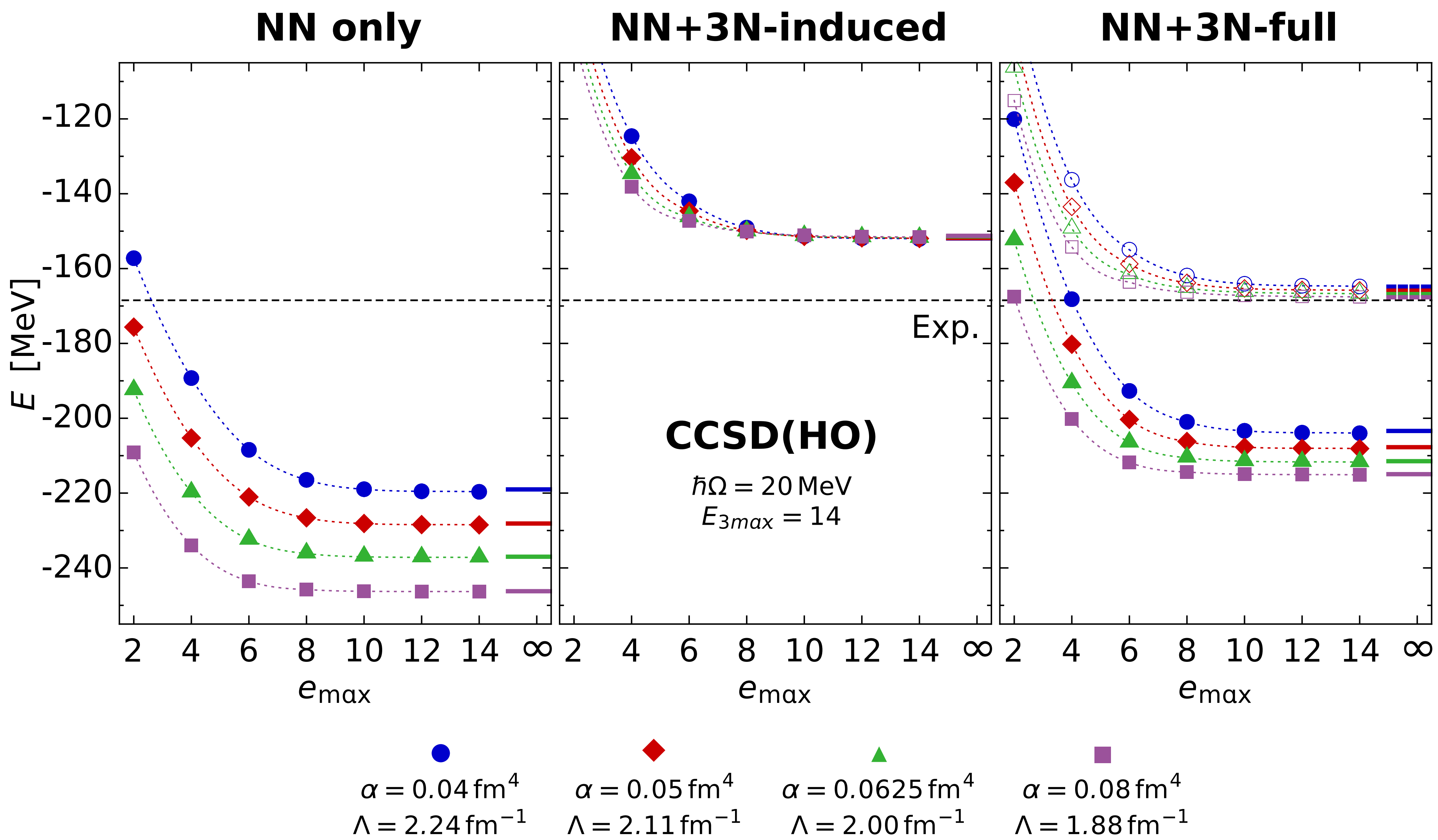
- **normal-ordering approximation** of the 3N interaction truncated at the two-body level
  - summation over reference state converts part of 3N interaction to zero-, one- and two-body terms

- both approximations are controlled and systematically improvable

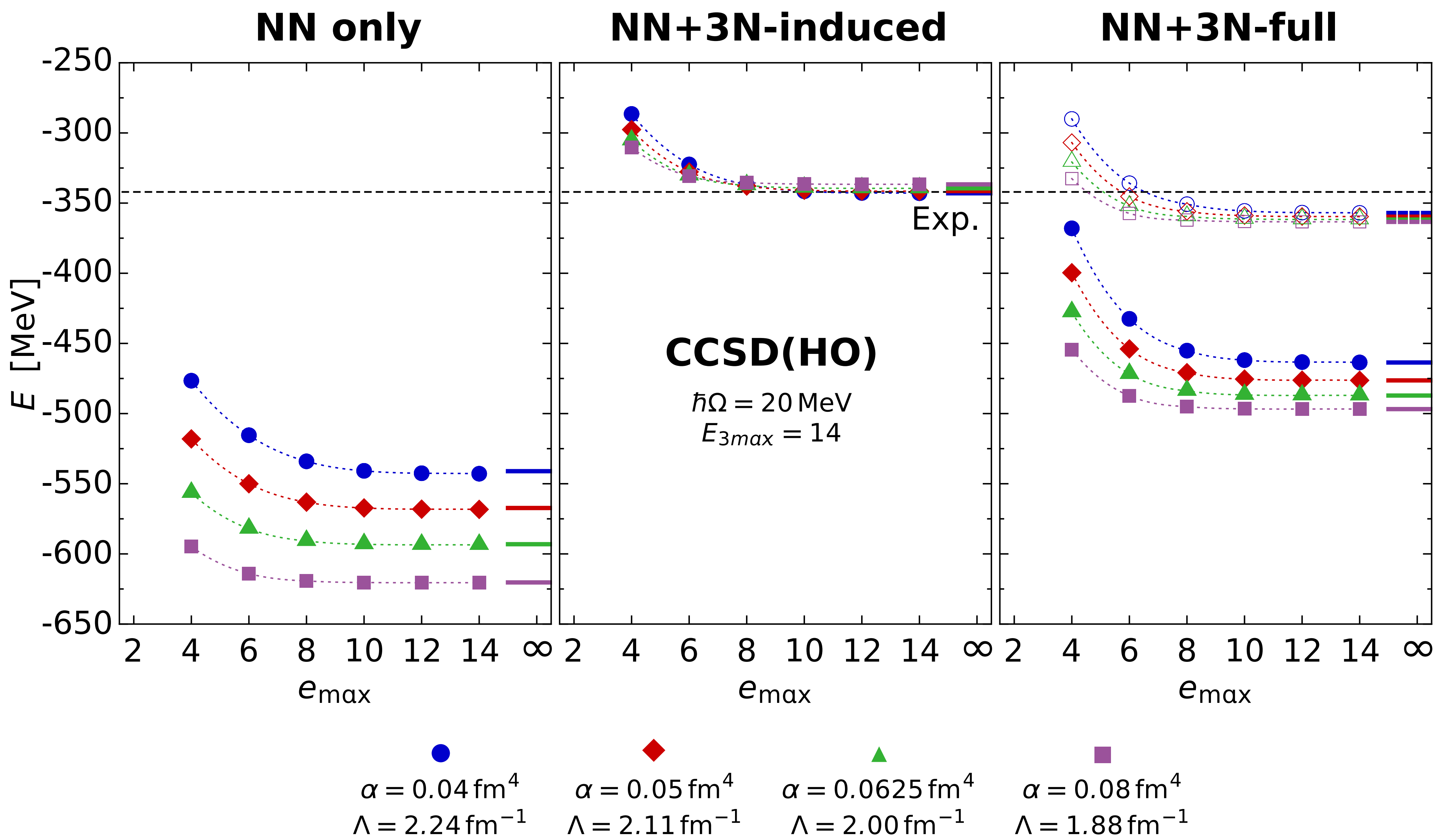
^{16}O: Coupled-Cluster with $3N_{NO2B}$



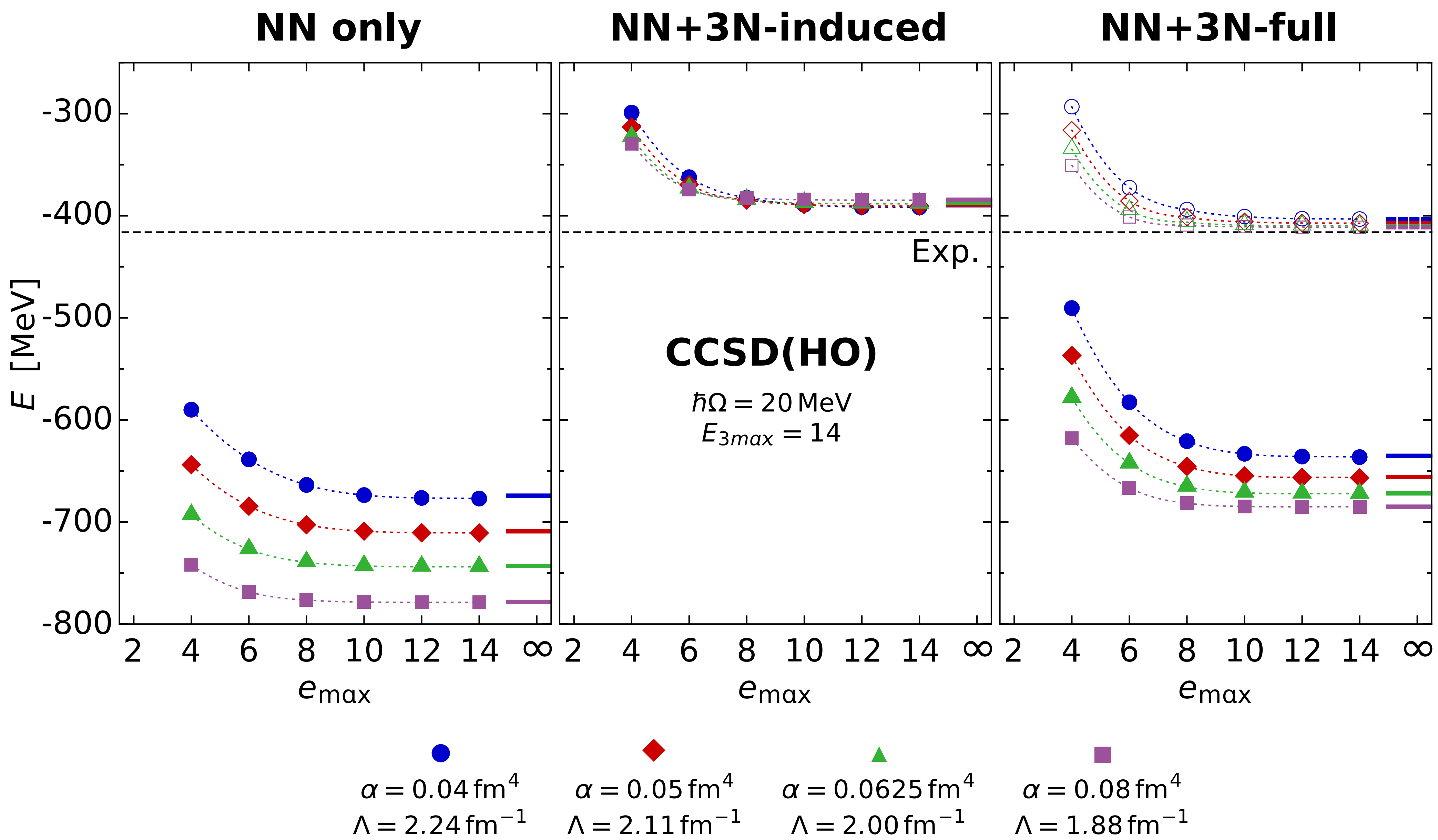
^{24}O: Coupled-Cluster with $3N_{NO2B}$



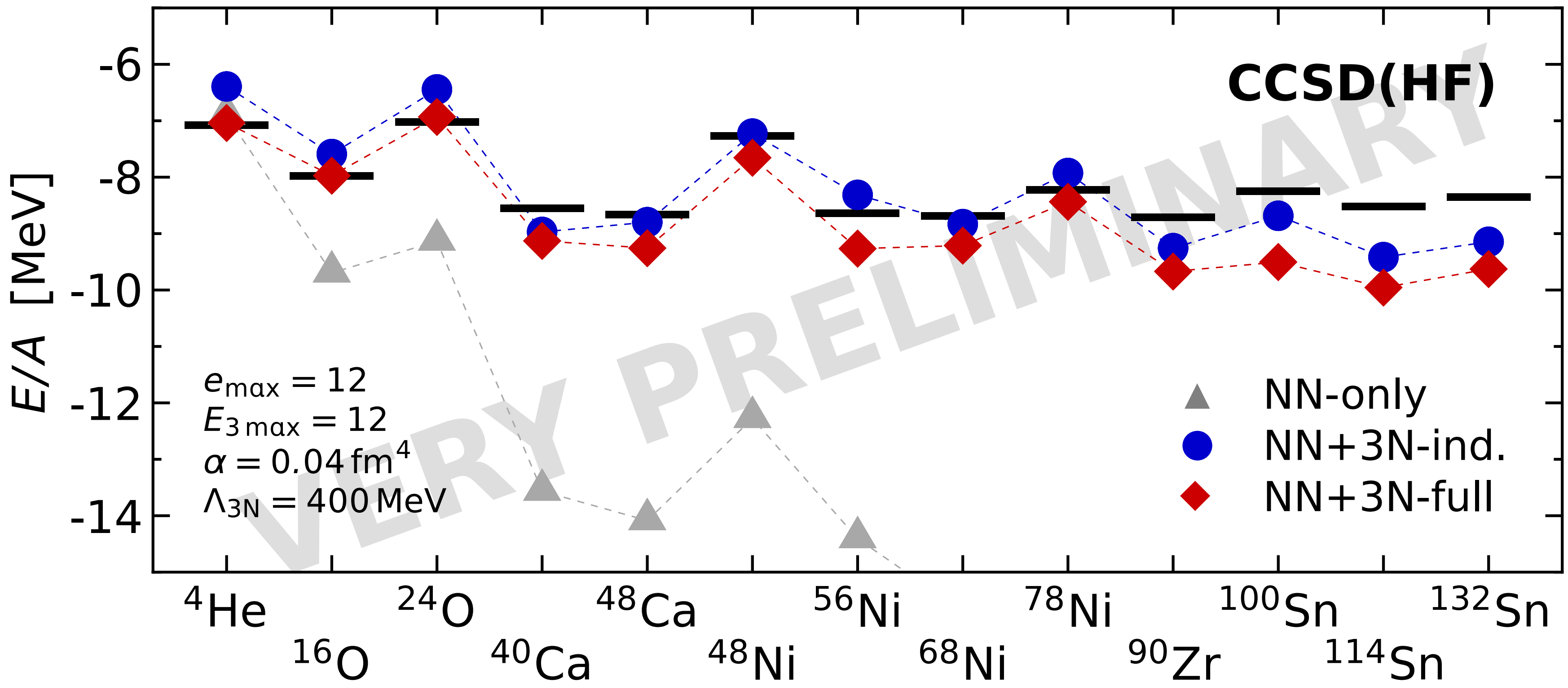
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



^{48}Ca: Coupled-Cluster with $3N_{NO2B}$



Outlook: Chiral 3N for Heavy Nuclei



- first ab initio calculations with **chiral NN+3N Hamiltonians for heavy nuclei**
- **realistic mass systematics** without phenomenological adjustments — α-dependence might hold surprises...

Conclusions

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some issues remain
- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
  - breakthrough in computation & handling of 3N matrix elements
- **innovations in many-body theory**: extended reach of exact methods & improved control over approximations
  - versatile toolbox for different observables & mass ranges
- many **exciting applications** ahead...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, E. Gebrerufael, A. Günther, H. Krutsch, **J. Langhammer**, S. Reinhardt, C. Stumpf, R. Trippel, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - J. Vary, P. Maris
    Iowa State University, USA
  - S. Quaglioni
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert, K. Hebeler
    Ohio State University, USA
  - P. Papakonstantinou
    IPN Orsay, F
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

JUROPA | LOEWE-CSC | HOPPER

COMPUTING TIME

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung